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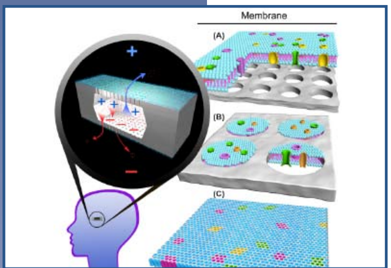
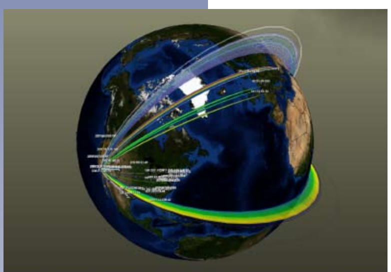
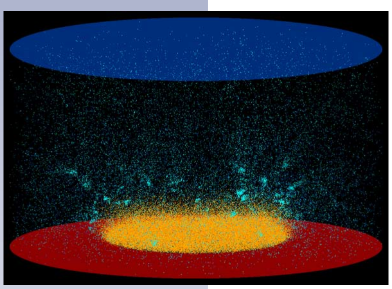
Science, Technology and Engineering



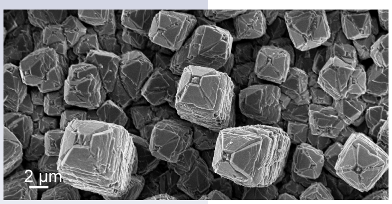
Bioscience



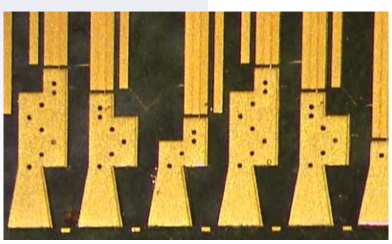
Computers and Information Sciences



Engineering Sciences



Materials Science and Technology



Microelectronics and Microsystems

Pulsed Power

Vision

Sandia National Laboratories is the provider of innovative, science-based, systems-engineering solutions to our Nation's most challenging national security problems.

Mission

Committed to "science with the mission in mind," Sandia creates innovative, science-based, systems-engineering solutions that

- sustain, modernize, and protect our nuclear arsenal,
- prevent the spread of weapons of mass destruction,
- provide new capabilities for national defense,
- defend against terrorism,
- protect our national infrastructures, and
- ensure stable sources of energy and other critical resources.

Guiding principles for ST&E

- Ensure that the fundamental science and engineering core is vibrant and pushing the forefront of knowledge
- Enable the programs by effective application of that science base
  - responding to current needs
  - anticipating the future

About *Science Matters!*

The purpose of ***Science Matters!*** is to publicize and celebrate recent Sandia accomplishments in science, technology, and engineering. We feature the science that underpins and enables technology for Sandia's missions. We nurture expertise, facilities and equipment to create world-class science that pushes the frontiers of knowledge and anticipates future mission needs. New ***Science Matters!*** are being issued semiannually.

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2/2009

Improving the Foundations of Complex System Modeling and Design

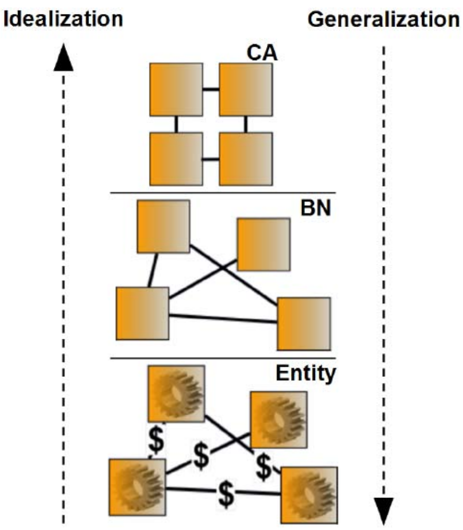

Figure 1: Various levels of complex system modeling. Squares: constituent entity models, idealized (plain) or realistic (with gears). Links: interaction paths (dollar signs for realistic interactions). From top: cellular automaton (CA) with homogeneous entities on a lattice; Boolean network (BN) with simple heterogeneous entities on a graph, limited to one-bit interaction; and general entity-based model with arbitrary interaction types.

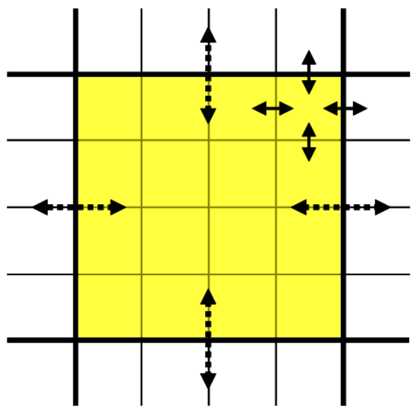

Figure 2: Schematic of renormalization in the case of lattice interactions. Initial entities interact with neighbors (solid arrows) on a fine lattice (light gridlines). A higher-level entity (entire yellow square) interacts with neighbors (dashed arrows) on a coarsened lattice (heavy gridlines), with the new interactions designed to preserve the system's large-scale behavior.

Complexity science has possible applications in cybersecurity

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Many complex systems that impact national security, such as energy infrastructure, terrorist networks, and the internet, differ from systems traditionally investigated in science and engineering by exhibiting intricate interactions among large numbers of entities that collectively display unpredictable emergent behavior. Emergent behaviors of complex systems, including self-organization and robustness, can be captured via simulation of interacting subsystems, an approach known as entity-based modeling. Absent conservation laws or an equation of motion, however, the construction of entity-based models is often *ad-hoc* and heuristic, more craft than science. Furthermore, the optimization of real-world simulations to achieve a desired behavior, such as making computers more secure or destabilizing a terrorist network, is often a matter of trial and error. The developing field of complexity science offers a new paradigm for modeling and design to complement traditional approaches. Through systematic studies relating models and emergent behavior at various levels of abstraction, Sandia's work in complexity science can guide the construction of entity-based models achieving a known or desired emergent behavior.

Complex systems evolve through networked interactions of their constituent entities and often exhibit emergent global behaviors that are not readily predictable from entity properties. To understand these behaviors, research at Sandia (in collaboration with MIT) has made use of idealized models such as cellular automata and Boolean networks. Insights obtained in these settings can be extended to more general entity-based models (Figure 1). Idealized computational studies have validated methods such as renormalization, a technique adapted from theoretical physics for constructing approximate coarse-grained models (Figure 2). Renormalization of complex system models provides a precise framework for understanding the abstraction process (the representation of lower-level entities by higher-level entities) that underlies practical simulations. The ability of renormalization to preserve certain emergent behaviors (Figure 3) suggests applications to more realistic complex systems.

Cybersecurity, the struggle to mitigate malicious intrusion into computer systems, is a national security challenge with a particular need for insights from complexity science. Due to the scale and sophistication of modern computer software along with classic mathematical results on undecidability, traditional engineering approaches have failed to curb the vulnerabilities of computer systems. Indeed, the practical impossibility of ensuring software correctness has given hackers an asymmetric advantage and led to a proliferation of malicious software exploiting the vulnerabilities (Figure 4).

Potential cybersecurity solutions drawing on complexity science are aimed at reversing this asymmetry. The interaction networks (physical or virtual) in a computer system can be studied in terms of coarse-grained models and emergent behavior; system characteristics that lead to global robustness can guide software design. Furthermore, compelling analogies exist to the naturally occurring complex systems of biology (as indicated by terminology such as computer viruses); genetics, evolution, and ecology can provide theoretical insights and practical strategies for mitigating threats. As Sandia tackles emerging mission areas, complexity science shows encouraging prospects for advancing cybersecurity and other national priorities.

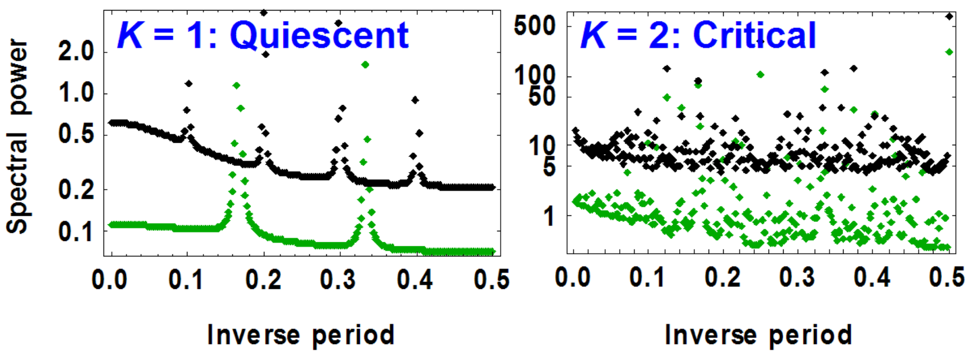

Figure 3: Comparison of emergent behavior of Boolean networks under renormalization. The initial Boolean networks are parameterized by *K*, the number of in-bound links to each node (entity). Plots show frequency spectrum of simulated dynamics for a 500-node initial graph (black points) and its 100-node coarsening (green points). The qualitative features distinguishing the "quiescent" and "critical" regimes are preserved.

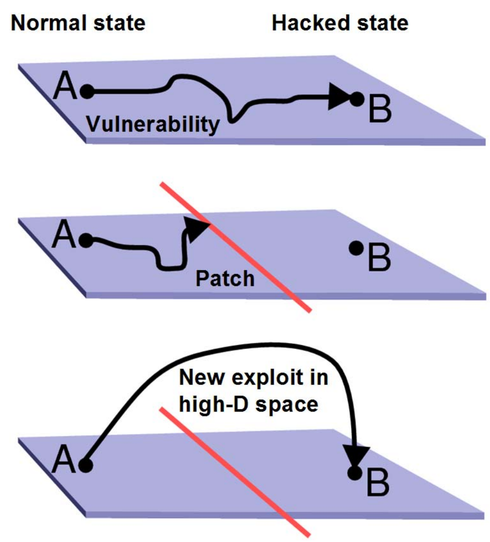

Figure 4: Origin of asymmetric threats to cybersecurity. A computer's vast state space defies complete verification; a vulnerability is quickly found and exploited (top). An analysis leading to a software patch (middle) can consider only a small subspace of states (violet slab). Other exploits act outside this subspace (bottom), thus turning current cyber defenses into "Maginot lines."

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Generating Contiguous Meshes for "Sloppy" Assembly Models

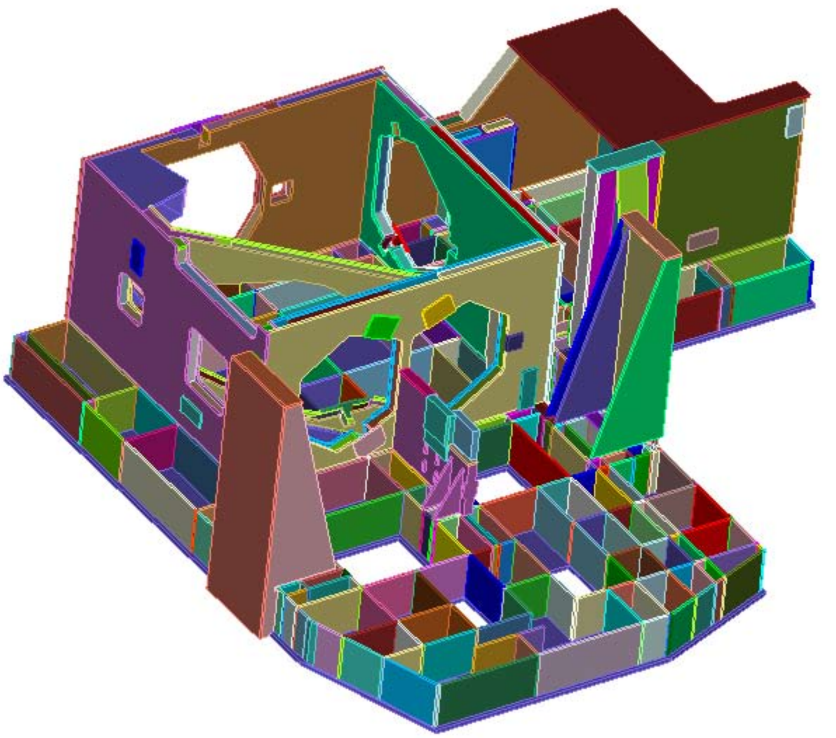

Figure 1: Example of CAD assembly model with hundreds of components.

Enhanced software speeds up analyses of complex weapons component assemblies

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Sandia regularly performs structural and thermal analyses on large nuclear weapon assembly models containing hundreds of components (see Figure 1). Since these analyses frequently require a discretized version, or "mesh," of the model, there is a need for software tools that automatically generate meshes. This is not a trivial task and has for many years been one of the main bottlenecks in the analysis process. Through advances in computational modeling, Sandia now has capabilities that have greatly reduced the amount of time required to generate meshes for large assemblies.

Many large assemblies contain "slop," or significant gaps, overlaps, and misalignments between assembly components. Slop may arise in a design from poor modeling practices or a mismatch in modeling tolerances between the original CAD (computer automated design) system and the meshing tool reading the input. Sometimes the models are accurate, but details such as press fit tolerances and adhesive layers must be removed under certain analysis conditions.

Meshes of assembly models are generally required to be contiguous across component-component interfaces. This means that two components that are in contact with one another in an assembly will share a mesh at the surface(s) of contact. Generating a shared mesh generally requires the CAD model to share surfaces between contacting parts. However, CAD models typically do not use this representation (often referred to as a "non-manifold" representation), and so it is necessary for the mesh generation package to generate a shared topology between parts before meshing.

The automatic recognition and creation of non-manifold connections between neighboring weapons assembly components requires the use of proximity checks to determine which components should be touching. If there are large gaps or misalignments between components, it is very difficult to determine if the design intent is for two components to be touching or not. This ambiguity generally complicates the process for automation as well as for manual intervention.

Thus Sandia has developed tools for generating non-manifold representations of CAD assembly models. These powerful tools are particularly helpful in the cases where there is significant slop in the CAD model that would normally require hours of manual geometry modification to fix. As shown in the flow diagram in Figure 2, improvements include tools to help the user identify the slop in the assembly, algorithms to automatically and tolerantly enforce criteria for creating non-manifold connections, and tools to analyze the results and identify remaining issues. For example, close proximities within the model now help determine the smallest allowable feature size. Then the largest allowable gap in the model is determined. Recent tests have shown an order of magnitude reduction in the number of manual geometric modifications required by the user when using these new tools. This equates to days saved in preparing a mesh for analysis.

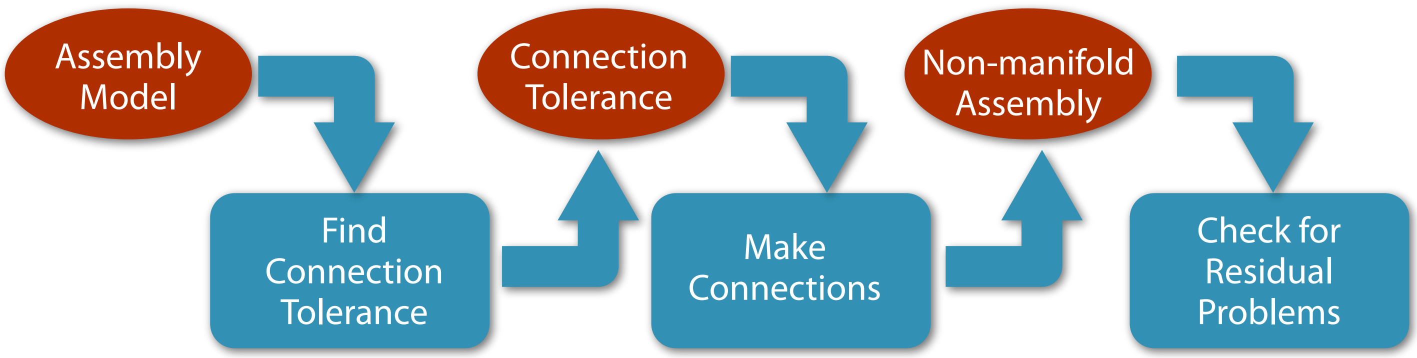

Figure 2: Flow diagram showing the process of generating connections in an assembly. The newly developed tools aid in the tasks highlighted by the blue boxes.

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Computer and Information Sciences
Computational Physics

Effectively Modeling Z-machine Wire Array Implosions

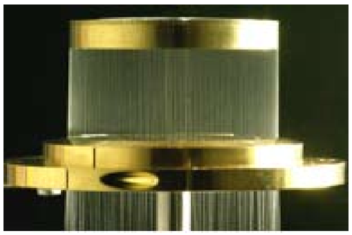

Figure 1: A wire array configuration used as a load for the Z-machine

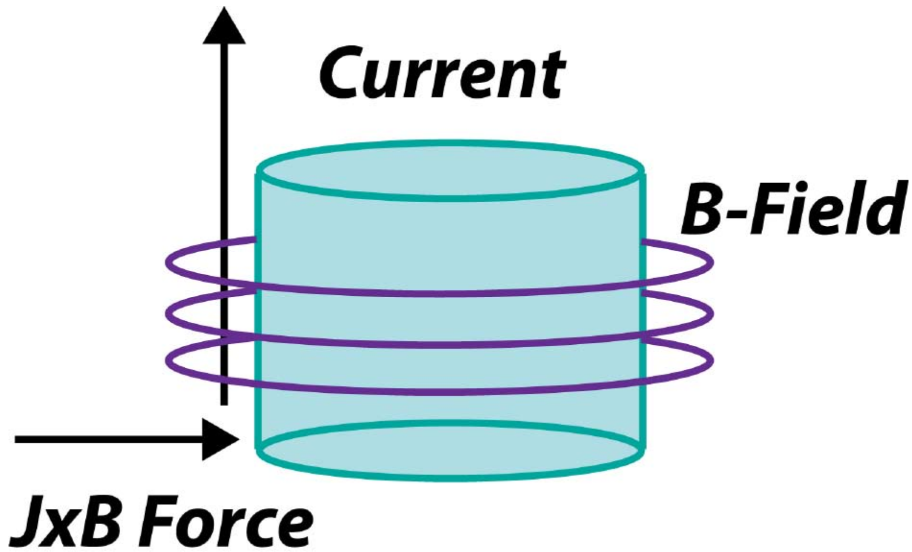

Figure 2: The current and associated magnetic field in the Z configuration drive a cylindrical implosion.

The ALEGRA magnetic-radiation-hydrodynamic code now has predictive capability for high energy physics

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The Z machine at Sandia characterizes high energy density matter under extreme environments. High magnetic fields are generated by wire-array implosions, where huge amounts of electrical current are run through a cylindrical array of tungsten wires (Figure 1). The magnetic field causes the wires to vaporize into a plasma and then drives the plasma toward the center axis of the array at high speeds (Figure 2). When this plasma stagnates at the axis, it generates considerable heat that exits the wire array as radiation. Modeling this highly energetic chain of events is enormously challenging because of the wide breadth of physics involved under extreme conditions.

Sandia's ALEGRA (Arbitrary Lagrangian-Eulerian) is a magnetic-radiation-hydrodynamic code that is designed to meet the challenge of modeling the wire-array implosion. ALEGRA has been around since 1994, but improvements in recent years have now enabled the effective simulation of wire-array implosions. A key enabling technology has been the implementation of a powerful solution to the magnetic portion of the problem using what are called compatible discretizations, which preserve the fundamental properties of magnetic flows exactly. In addition, codes like ALEGRA typically solve for the energy of the flow concentrating on the thermal content of the fluid. The problem is that flows like those found in a wire array are dominated by the energy of the magnetic field or the motion of the flow for significant portions of their evolution.

In fact, the process where the energy of the motion comes to a halt is critical (i.e., when the flow hits the center axis of the wire array and is converted into heat). Therefore, Sandia had to modify the solution for the energy of the flow to more accurately account for this process and to rearrange the energy accounting in the flow so that it also could be accurately simulated.

With the utilization of the new methods in ALEGRA, in combination with an innovative

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technique for modeling the vaporizing wire array, it was discovered that one could now simulate wire-array implosions with enough accuracy that they could be compared favorably with experimental data (Figure 3). Furthermore, ALEGRA could be used to analyze and design follow-on experiments because of this predictive capability. This provided the scientists working on experiments in the Z-machine with new-found confidence in the predictive power of the simulations with ALEGRA.

Sandia continues to improve the algorithms by careful development and detailed analysis. A similar method has been developed for conserving magnetic energy as material moves through the computational mesh. Impressive improvements in shock test problems are observed by accounting for this energy (Figure 4).

References

R. Lemke, et al., "Effects of Mass Ablation on the Scaling of X-Ray Power with Current in Wire-Array Z Pinches," 16 January 2009 issue of *Physical Review Letters* (Vol.102, No.2): DOI: 10.1103/PhysRevLett.102.025005

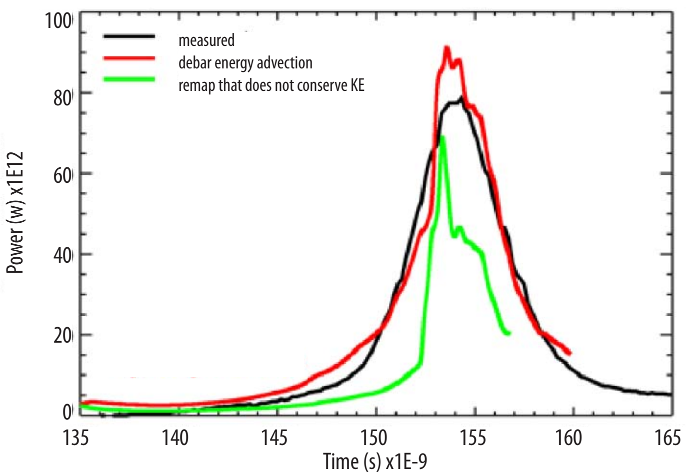

Figure 3: Algorithms to ensure that kinetic energy is preserved with material motion allow for vastly improved comparison with data.

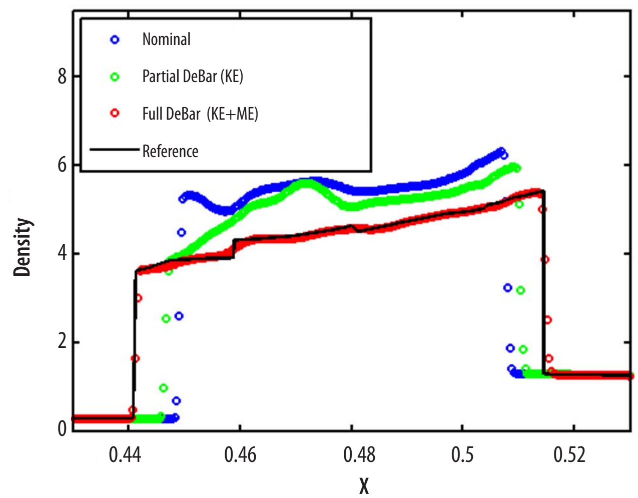

Figure 4: Magnetic energy conservation algorithm with material motion shows that additional quantitative jumps in solution accuracy are possible.

Informatics for Network Discovery, Prediction, and Disruption

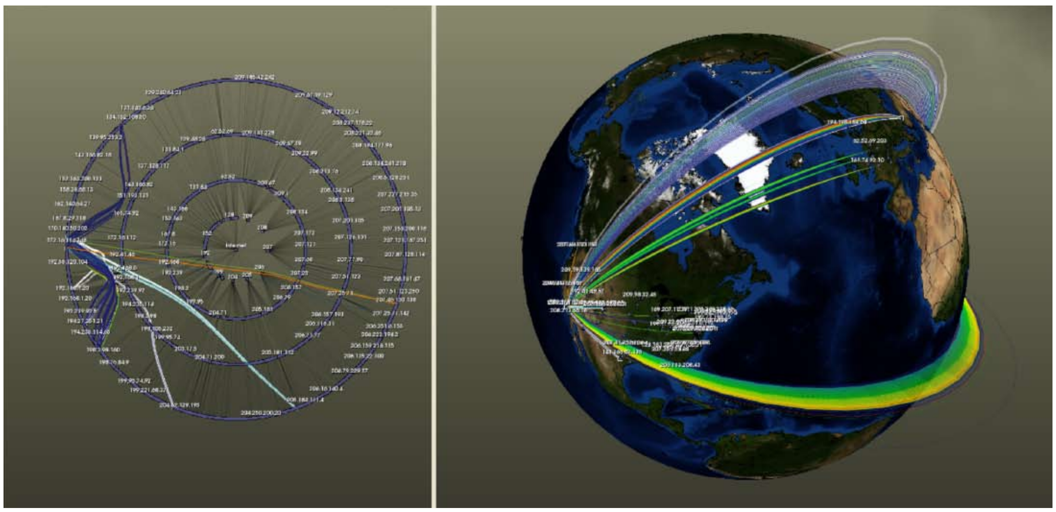

Figure 1: Depiction of network file transfers between computer IP addresses (show as arcs in the ring-view on the left), and network file transfers crossing country boundaries (shown as arcs in the geospatial view on the right).

Transformational methodologies are needed to ferret out the security threats buried within massive amounts of benign information

Informatics is the science that encompasses complex information and relationship-based analytic methods to support decision-making in uncertain and massive-data environments. Sandia is carving a unique niche and positioning itself as a leader in solving complex and large-scale informatics problems, especially those involving national security. To that end, Sandia is building a strong research program that utilizes many distinguishing laboratory strengths: discrete math, fast graph analytics, alternative data machines, linear algebra methods, information visualization, computer architectures, high-performance computing, and scalable algorithms.

Terrorist networks, like social networks, are a good example of complex relationships that challenge informatics capabilities. People can be described in terms of their human attributes, the characteristics of their activities, and the interrelationships between their activities which connect them to others. When people engage in suspicious activities that threaten national security – through networks of adversaries engaged in weapons proliferation, terrorism, cyber attacks, and other illicit activities – and when these adversarial networks in turn hide their activities among the complex interactions between legitimate and illegitimate secondary networks (e.g., for communication, computing, supply chain, and financial transactions), then transformational methodologies are needed to ferret out the threats buried within massive amounts of benign information.

Math and computer science researchers in informatics have teamed with mission-driven analysts and experts in uncertainty quantification and human factors to focus on decision-making in complex national security environments. One research project in particular focuses on informatics for discovery and prediction. A sub-team on that project recently demonstrated a thin slice of end-to-end capabilities in a prototype targeting cyber analysis in computer networks. Using fabricated network traffic test data supplied by MIT Lincoln Labs, the sub-team processed raw data and analyzed it to answer four postulated questions: 1) What computers

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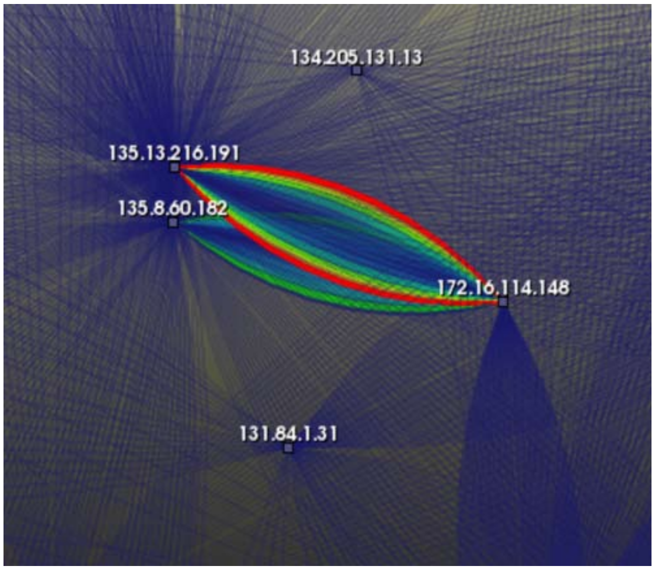

Figure 2: Example of information visualization with brightly colored arcs to highlight suspicious network activities. "Normal" network traffic fades visually when represented as dim blue arcs.

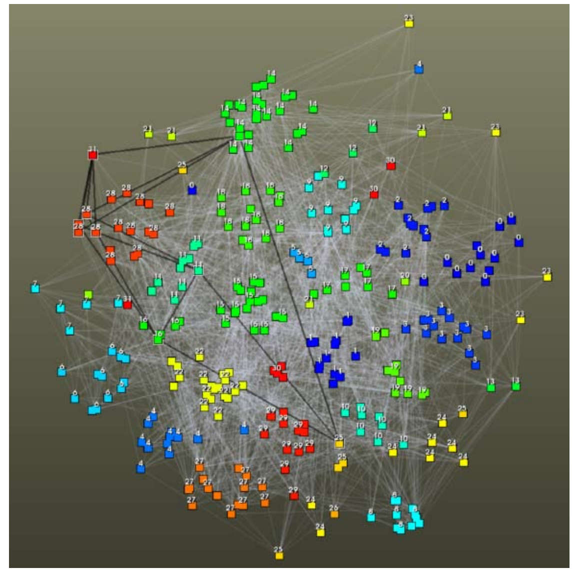

Figure 3: Powerful graph searches are used to cluster and aggregate related information (shown as commonly colored groupings). Connection sub-graphs depict multiple paths between two nodes in a graph (e.g., lines between upper left red node and lower right yellow node).

were communicating with each other? 2) What network file transfers crossed country boundaries? 3) What information was contained in the transferred files? 4) What suspicious network activities occurred? Figure 1 depicts several linked visualizations that answer question #2. The ring-view (left) shows successive rings of computer networks, sub-networks, and individual computers (white IP addresses) exchanging files across the Internet. The geospatial view (right) integrates an IP address lookup function to show the countries of origin and receipt where the computers reside. The example leverages scalable data queries with analytical graph searches and visualization for presentation to the analyst.

Figure 2 also shows how information visualization can quickly depict unusual or suspicious behaviors that need further investigation (question #4). All the "normal" and expected traffic fades to the background visually (as dim blue arcs), while the suspicious traffic is highlighted in a rainbow of colors where each color represents a different form of network activity between two computers (like file transfers). This helps the analyst to focus on the small subset of larger network traffic to answer whether the suspicious activities are legitimate or illegitimate. The scenario applies conditional statistics to the results of a data query before visualizing the results of the graph search. Figure 3 shows the results from powerful graph searches used to cluster and aggregate related information: finding and identifying communities (groups of colored squares) and finding connected sub-graphs that give multiple paths (black lines) between two specific nodes (upper left red and lower right yellow).

Sandia has begun to address the design of an overall distributed systems architecture, targeting large informatics applications, that leverages the capabilities of different computers to perform the tasks that each does best: data machines for database searches, multi-threaded machines for rapid graph queries, client-server architecture for delivery of visual outputs to user-analysts, and high-performance computing and distributed memory machines for math computations. In a recent success demonstrating part of a distributed systems architecture, Sandia was able to link data accesses on a Netezza data machine with visual analytics running on the Red Storm high performance computer (Fig. 4). The early prototype and systems architecture design are positioning Sandia to analyze informatics problems of unprecedented scale and complexity.

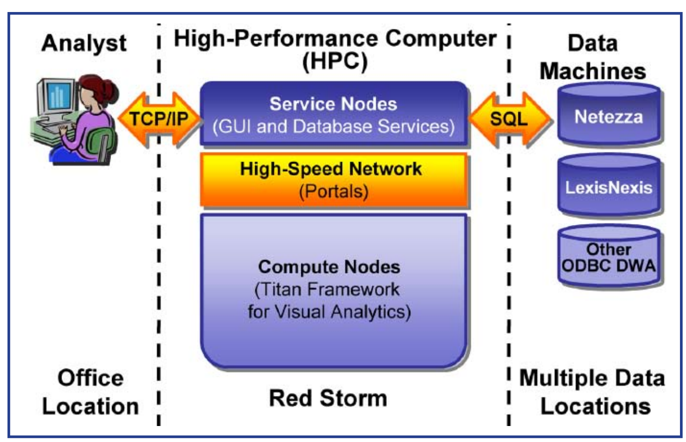

Figure 4: Distributed Systems Architecture: An analyst sitting at her workstation can run a high-performance computing (HPC) application on the Red Storm computer. The distributed systems architecture enables the HPC application to leverage remote data warehouse appliances (DWA) for efficient data access and management.

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Consistent Modeling of Discrete and Continuous Mechanics

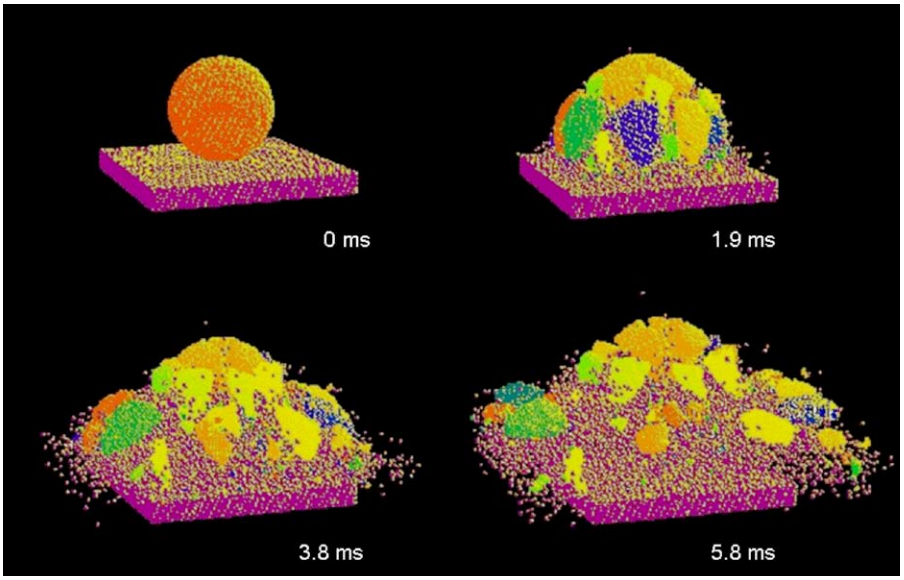

Figure 1: Because the peridynamic theory can treat any number of mutually interacting dynamic fractures, it provides a natural way to model fragmentation. This computer calculation reproduces fragmentation due to the impact of a brittle sphere against a rigid wall.

Peridynamics could lead to higher fidelity in physical simulations and provide a new pathway to the goal of multiscale modeling of materials

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Many researchers have attempted to couple the standard differential equations of continuum mechanics with discrete models for atomic and molecular systems. There have also been many efforts to couple models for crack growth with models for continuum mechanics. What these efforts have in common is that they try to connect mathematical systems that are fundamentally dissimilar from each other: one set of equations for the continuous model, and another for the discrete. This leads to the need for complex and sometimes problematic coupling techniques.

Sandia researchers have asked the question: What would happen if, instead of coupling dissimilar mathematical systems, the same physical phenomena could be modeled within a single, consistent set of equations? These same equations would be applicable everywhere in a body, regardless of whether it is treated as a set of discrete particles or as a continuum, and regardless of whether cracks or localizations form. The hypothesis is that such a mathematically consistent model could lead to higher fidelity in physical simulations and could provide a new pathway to the goal of multiscale modeling of materials.

The method involves developing a new theory of continuum mechanics called the *peridynamic* model. This theory treats discrete particles, fracture surfaces, and continuous bodies all with exactly the same equations. It accomplishes this by using integral equations rather than partial differential equations. Mechanically, the integral equations represent direct interactions between points in a body within a predefined distance of each other, called the horizon. The peridynamic model does not use stress and strain; these are concepts that are important in the standard theory, but which hinder application to discrete systems. Instead, the Sandia model characterizes the internal forces within a body in terms of force densities between points in a body. The model therefore has a natural similarity to molecular dynamics. Figures 1 and 2 illustrate some of the advantages of the peridynamics model.

A number of significant accomplishments have emerged from this effort: (1) In the limit as the horizon approaches zero, it was proved that the peridynamic equations converge to the partial differential equations of the standard theory. In this sense, the standard theory is a subset of the peridynamic theory. (2) It was shown that a set of discrete classical particles, such as atoms interacting through a multibody potential, can be modeled exactly as a peridynamic body. (3) The notion that the integral equations of peridynamics can be obtained from statistical physics was also demonstrated. (4) A peridynamic energy equation that contains a more general notion of work conjugacy than in the classic theory was derived. (5) Sandia implemented the peridynamic model within LAMMPS, its widely used molecular dynamics software.

The expectation is that these recent advances will enable Sandia to use the peridynamic theory as a mathematically consistent framework in which to coarse-grain atomistics into a continuum model.

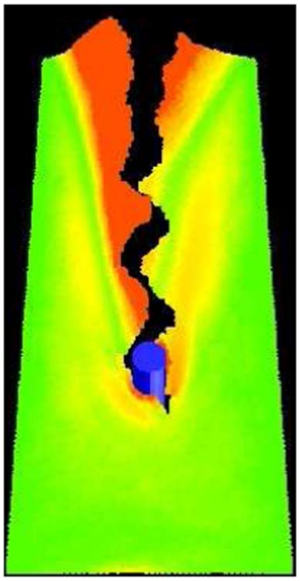

Figure 2: Mathematically consistent treatment of discontinuities reveals subtleties in the mechanics of fracture. Here, a peridynamic simulation reproduces the instability that results in a wavy crack trajectory in a membrane pulled past a rigid cylinder.

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02/2009

Engineering Sciences
Microscale Science

FemtoNewton-Scale Colloidal Force Measurement using Optical Trapping

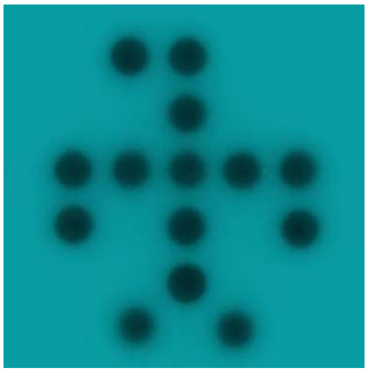

Figure 1: Laser tweezers optical trapping is used here to manipulate silica microparticles into a Sandia thunderbird.

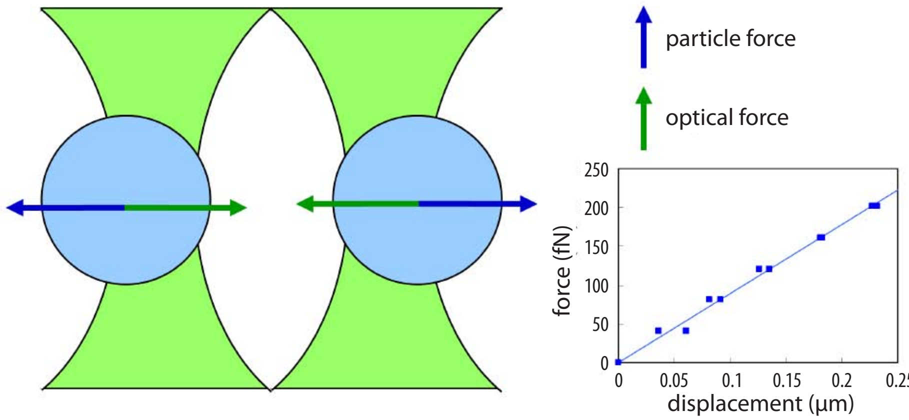

Figure 2: Diagram of the direct force technique to measure forces between colloidal particles. If a particle feels a repulsive force from a nearby particle, it will be pushed out of the center of the optical trap. By looking at the equilibrium position of the particle, we can determine the colloidal force from the known restoring optical force.

The ability to measure tiny forces between particles has widespread applications in nanotechnology and biology

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Optical manipulation of small objects using focused laser light was pioneered by Arthur Ashkin, and has found wide-spread application to both biological and physical sciences. By harnessing light's momentum, objects from neutral atoms to living cells can be trapped in three dimensions (Figure 1). Laser-based optical trapping has also been used to measure weak forces between small charged microparticles such as colloids. At Sandia, the extremely weak femtoNewton (fN, 10^{-15} N) forces between two colloidal particles have been measured by using two independent implementations of optical trapping for the first time.

The first technique, "direct force," relies on knowing the force required to hold the particle in the center of the optical trap. Once this restoring force is calibrated, one can measure other external forces applied to a trapped particle by monitoring its position relative to the center of the optical trap. As shown in Figure 2, when two trapped particles are brought close to each other, the displacement from the trap center for each particle increases proportionally to the interaction force. The full range of inter-particle forces is determined by gradually moving the two trapped particles closer together.

The second technique, "blinking laser tweezers," takes advantage of the natural thermal diffusion of colloidal particles. Two particles are held near each other and then the optical traps are turned off. The particles then move due to random Brownian motion and any other applied forces. By repeatedly catching and releasing a pair of particles, one can gather physical statistics of many particle trajectories (Figure 3). Statistical analysis is used to determine drift velocities, diffusion coefficients, and ultimately colloidal forces as a function of the center-center separation of the particles. The optical traps allow the particles to come into energetically unfavorable separations which are frequently found in flows of concentrated colloids. Also, since the measurements are made while the

lasers are turned off, there is no risk of optical forces or induced dipoles affecting the measured forces.

Both approaches were used independently to examine the forces in a model system of polystyrene microparticles suspended in hexadecane with 1mM AOT (dioctyl sodium sulfonsuccinate, a surfactant used as a charge control agent). As shown in Figure 4, the forces are measured, using both direct force and blinking techniques, as a function of the distance between two particle surfaces. At large separations, their electrostatic repulsion is completely screened by the surrounding fluid and there is no measurable force. As the particles approach each other, the repulsive electrostatic force between them increases rapidly in a form well represented by Derjaguin-Landau-Verwey-Overbeek (DLVO) theory (black line). The two methods agree quantitatively and have a force resolution of 30 fN.

Currently, these measurements of weak interaction forces are enabling predictive simulations of nanoparticle dispersion flow and stability for Sandia's Nanoparticle Flow Consortium. Optical manipulation is also being used to build novel particle structures with potentially unique optical properties. Future applications of the optical trapping methods include force measurements in biological systems, such as those occurring between cells or liposomes, in to order to understand their interaction with surfaces and each other as well as conditions required for membrane fusion.

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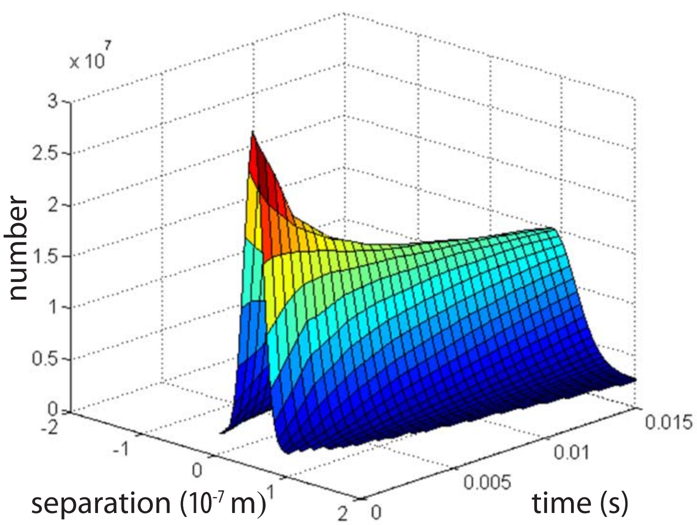

Figure 3: Blinking laser tweezers results showing histograms of particle separation as a function of time. As time passes after the optical traps are turned off, the distributions broaden as the particles diffuse around due to random Brownian motion. The central peak of the distributions also shifts to larger separations due to electrostatic repulsion. The particle diffusivity and mean velocity are used to calculate the force between the particles.

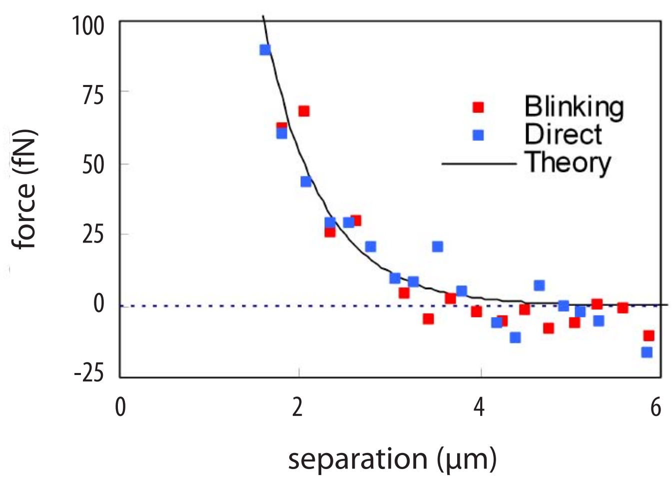

Figure 4: Measured interparticle force as a function of particle separation between two polystyrene particles in a hexadecane–AOT solution. The comparison is quantitative and well-represented by DLVO theory.

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National Nuclear Security Administration

02/2009

Engineering Sciences
Plasma modeling

Zap, Crackle, Pop! Simulating Arc Discharges

New codes will reveal the details for electrical arc initiation and evolution

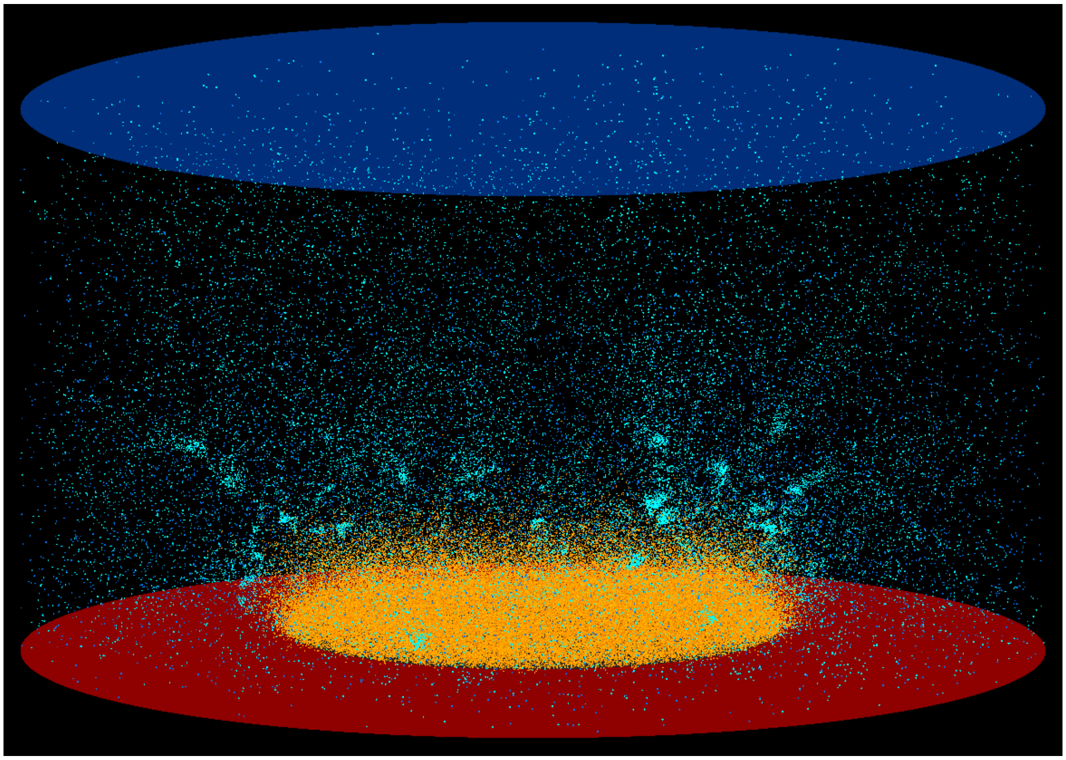

Figure 1: Electrons (blue) from a "virtual" cathode at top have heated the bottom anode, generating a tremendous number of neutral titanium atoms (orange). Some of these in turn have been ionized by electrons, producing titanium ions (light blue). Note the localized multiple ionization events.

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Arc discharges are encountered all the time, every day. Spark plugs in a car, static discharge with a doorknob, fluorescent lighting, and atmospheric lightning all operate according to similar principles. Yet there is no predictive model for their initiation and evolution suitable for the advanced design and engineering tasks performed at Sandia (with increasing frequency). Thus over the past two years, there have been efforts to develop new models within the Aleph low temperature non-continuum plasma simulation tool to help understand arc discharge initiation and evolution. Although the primary motivation is to understand plasma arc discharges in neutron tubes, these models apply to other discharge events, including other arc-based devices.

An arc discharge in an electrode-based system begins with electrons traveling from a cathode to an anode due to a voltage drop across the gap. The incoming electrons heat up the anode; when it gets very hot, the anode releases neutral atoms (see Figure 1). As it gets hotter and hotter, more and more neutral atoms are released from the anode. Occasionally, an electron and neutral atom collide or interact strongly enough to ionize the atom by knocking off one of its outer electrons. Thus, one electron and one neutral atom are converted into two electrons and one ion. If the conditions are just right, those two electrons now have the opportunity to ionize more neutral atoms, etc., leading to a very rapid increase in ionization rate called an "electron avalanche" or a "cascade event."

In other words, an "arc" is formed. The arc persists as long as the drive conditions and source materials are available. In this simplified description, many details are omitted that are necessary to realistically model how arcs form. Much of Sandia's research effort is spent digging through those details, constructing models based on them, and testing them within the Aleph code.

A simulation exhibiting some of these events as a function of time is shown in Figure 2. Only a small fraction of the actual particles in the simulation are displayed. The lower surface contains the anode (center disc). However, unlike the above description, we do not have an actual cathode in the simulation. The upper surface is simply emitting a constant stream of electrons, acting as a "virtual" cathode. The electrons travel to the anode, where their energy is deposited and heats the material. The temperature is tracked, and a desorption (vaporization) model is used to emit neutral titanium atoms. Those atoms diffuse away from the surface, and occasionally one is ionized by an incoming electron, producing titanium ions. Cascade-like events can clearly be seen.

A fully developed predictive arc simulation tool will improve our scientific understanding of the initial plasma breakdown event. In addition to pure scientific understanding, a predictive tool will also allow us to perform device optimization and uncertainty quantification. These advanced design and engineering processes lead to reduced costs, shorter design and analysis cycles, and overall higher quality and confidence in product performance. We have made great progress in the first two years, but still have much to discover and learn.

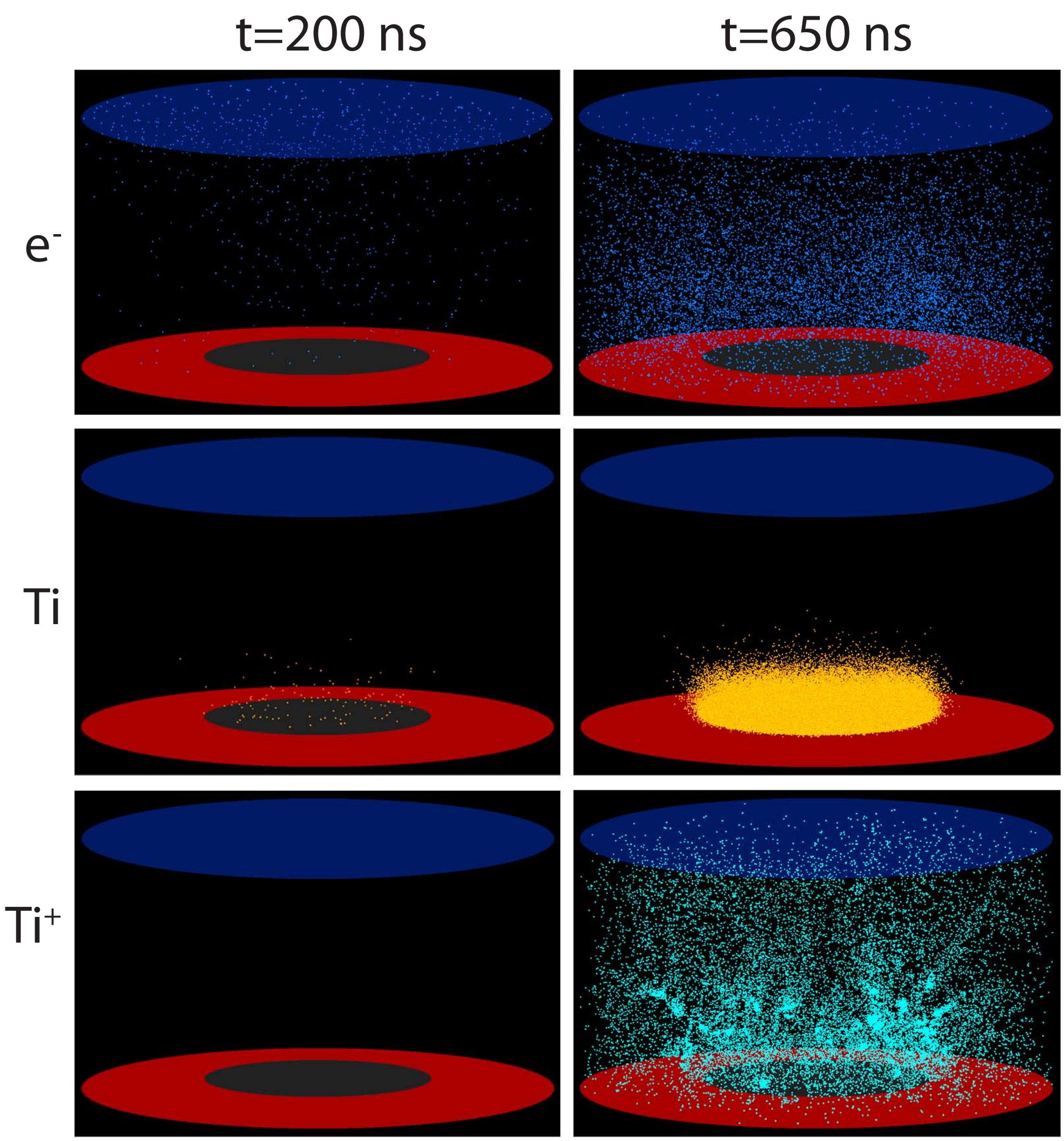

Figure 2: Evolution of arc initiation over time. At 200 nsec, the anode has been heated only slightly, emitting some neutral titanium atoms. At 650 nsec the greatly increased heating of the anode leads to the generation of many more neutral titanium atoms, and thus a much higher ionization rate. Note in particular some cascade-like ionization events.

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02/2009

Materials Science and Technology
Composites

Metal-Organic Frameworks

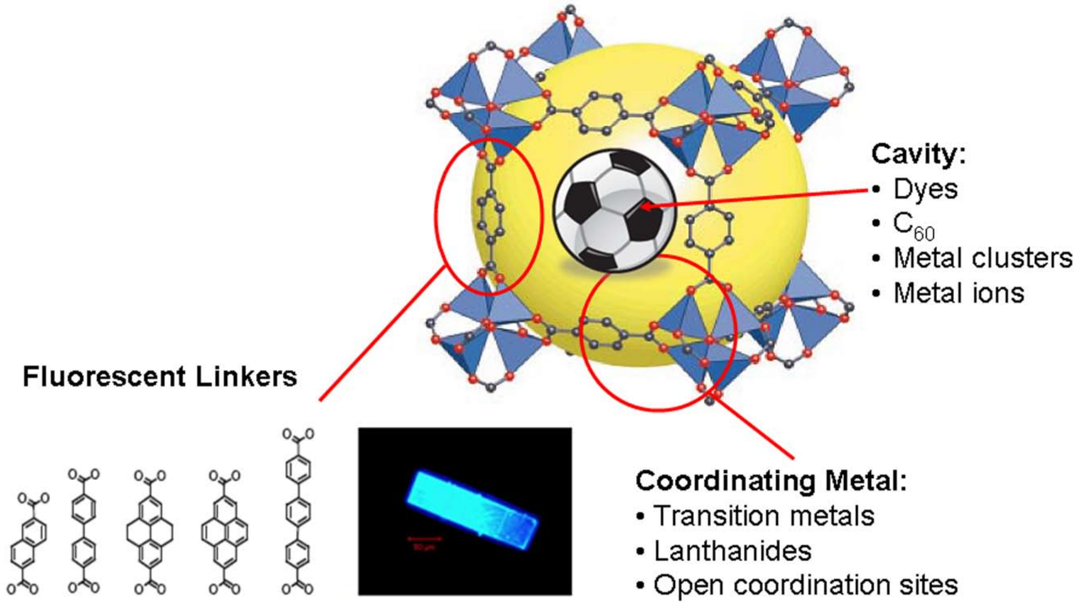

Figure 1: Potential sensing mechanisms in a typical MOF, illustrated using the classic MOF-5. This consists of Zn(II) ions (at the center of the blue tetrahedrons) linked by benzene dicarboxylate groups (black dots: carbon; red dots: oxygen). The yellow sphere represents the open space available for guest molecules.

Versatile nanoporous materials can be designed for diverse sensing applications

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The need for real-time, compact, and inexpensive sensors continues to grow in both complexity and urgency. Homeland security and defense applications such as portal monitoring, chemical weapon detection, radiation detection, and water quality monitoring have long been high priorities. Other newer applications include personal exposure monitors, sensors to provide advance warning of food spoilage, and breath analyzers that provide pre-symptomatic indication of infection. Development of these systems can be very demanding in several ways, requiring high levels of sensitivity and specificity in small, economical packages.

Novel nanoporous materials known as metal-organic frameworks (MOFs) are currently attracting considerable attention for a variety of sensing applications. They are ideal candidates because they have tailorable nanoporosity and ultrahigh surface areas. A typical MOF (Fig. 1) consists of metal cations such as Zn(II) linked by anionic organic groups such as carboxylates, yielding a rigid, open framework with cavities that can accommodate guest molecules. The metal ion framework can have open coordination sites to accommodate ligand binding. The organic linkers can consist of a variety of functional molecules, including fluorophores. The versatility of the combined framework and linkers allows these materials to function as sensors in a variety of ways, two of which are discussed below.

In the first example, a sensor is designed to take advantage of MOFs that can alter their unit cell dimensions by as much as 10% when guest molecules are adsorbed within the pores. Gas adsorption will therefore cause distortions in a supported thin MOF film. This creates a novel transduction mechanism if, as depicted in Fig. 2, the substrate is a microcantilever that bends under interfacial stress. Thus the gas adsorption is detected via the stress-induced bending of the microcantilever that can be monitored by a very sensitive optical sensor or by a built-in piezoresistive stress sensor. Recently, this was demonstrated with a copper-containing MOF (Fig. 2). In its hydrated state, the MOF layer enables water vapor, methanol, and ethanol vapors to be detected to varying extents, with no response to N_2, O_2, or CO_2. In contrast, removing water bound to exchangeable sites on the MOF, as well as adsorbed within its pores, turns on sensitivity to CO_2. Thus MOFs can serve as effective recognition chemistries for a variety of gases and might be useful in a breath analysis or humidity sensing application.

In a second, very different, example, new MOFs containing the organic fluorophore stilbene dicarboxylate as a linker emit visible light on nanosecond timescales when irradiated with high-energy protons, alpha particles, and electrons (Figure 3). A completely new class of scintillation materials is created by this development, with the potential to rationally tailor properties for specific radiation detection applications. In general, the detection and identification of subatomic particles is an important scientific problem with implications for medical devices, radiography, biochemical analysis, particle physics, nuclear nonproliferation, and homeland security.

These two examples demonstrate that MOFs are indeed multifaceted. There are, however, many other MOFs that remain largely undeveloped as sensing materials. Research at Sandia therefore aims to realize this potential by both understanding the underlying mechanisms for sensing and by developing methods needed to integrate them with other materials and devices.

Figure 2: MOF-coated microcantilevers can be used to detect a variety of gases. In this case, the crystal lattice of the MOF CuBTC (copper ions linked by benzene tricarboxylate groups) expands or contracts when it adsorbs an analyte, creating measurable stress at the interface with a microcantilever.

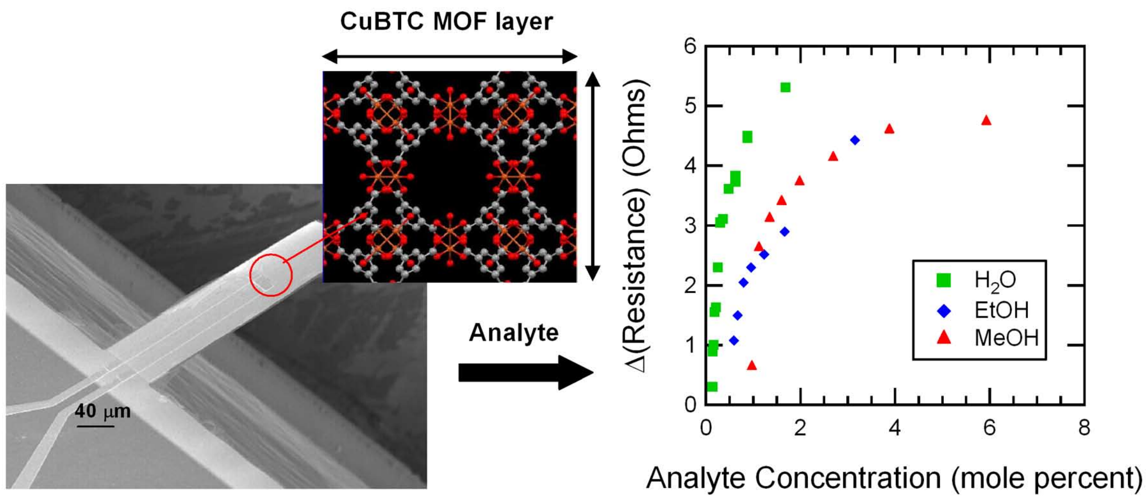
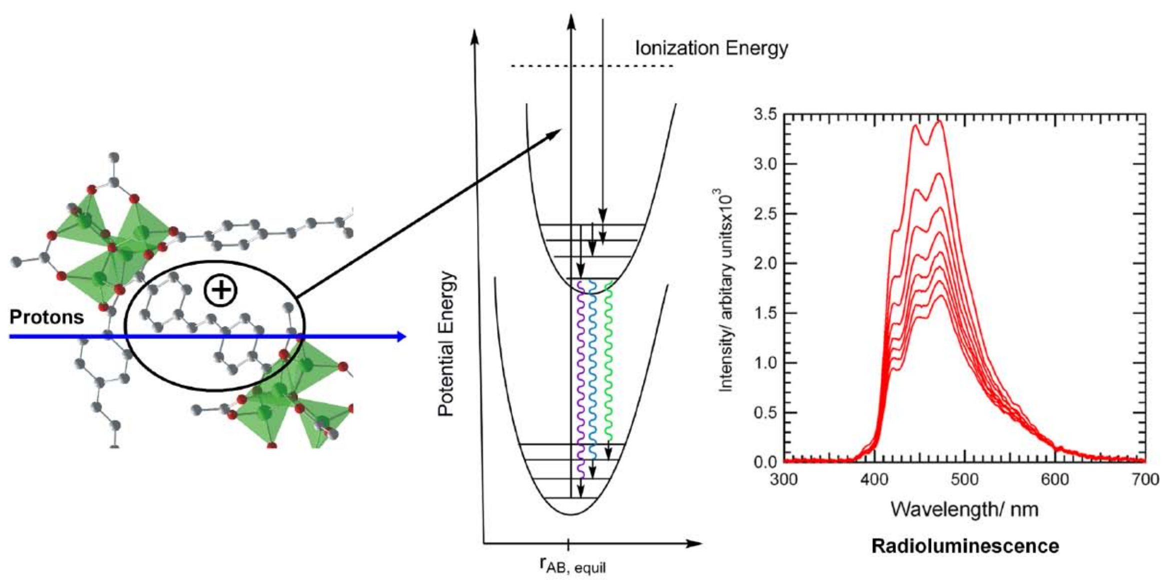


Figure 3: Schematic of scintillation induced by high-energy protons in a MOF.



Materials Science and Technology
Nanoscience

Fabrication of Large-Area 3D Nanostructures

Proximity-field nano-patterning lithography can produce nanostructures over large areas using a simple optic and a single cycle of lithography

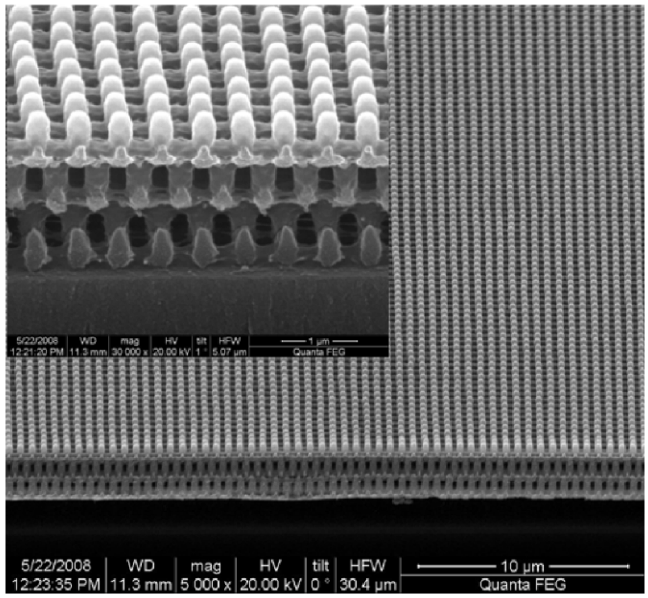


Figure 1: Example of 3D nanostructure made by the PnP method with a periodic square array.

Three-dimensional (3D) nanostructures are vital for emerging technologies such as photonics, sensors, fuel cells, catalyst supports, and data storage. Conventional fabrication (repeated cycles of standard photolithography with selective material removal) is costly, time-consuming, and produces limited geometries. Unconventional methods (colloidal self assembly, template-controlled growth, and direct-write or holographic lithography) have uncertain yields, poor defect control, small areas, and/or complicated and costly optical equipment. The Proximity-field nanoPatterning (PnP) method overcomes these limitations by generating complex 3D nanostructures using a simple optic and one lithographic exposure and development cycle. The optic is an elastomeric "phase mask" patterned in 3D dimensions roughly equal to the exposure wavelength. The phase mask is laid directly onto a spincast photopolymer and the light intensity pattern exposes the photopolymer in certain regions. Light exposure through the mask generates a complex 3D light intensity distribution due to diffraction and the Talbot effect. The exposed photopolymer is baked and developed, producing a 3D network of nanostructures with a single lithography cycle (Figure 1).

The PnP process has been transferred to the Sandia microfabrication facility, and scaled-up to produce 3D nanostructures across a full 6-inch wafer, thus making potential integration with microelectronics and microsystems possible. Modification of the photopolymer with solid reactive diluents has led to reduced structural shrinkage (due to chemical cross-linking that occurs upon post-exposure baking); while modification with conjugated organic dyes has led to the use of wavelengths outside the normal range (>500 nm). The 3D polymer nanostructures are fairly robust, but lack the materials characteristics desired for photonic applications. To alleviate this problem, a graded temperature approach was developed for atomic layer deposition to coat the 3D

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structures with dielectrics (Al_2O_3, ZnO, TiO_2) and metals (Pt), thus modifying the chemical, surface, and optical properties.

To predict the phase mask required to generate a specific desired nanostructure, a Finite Difference Time Domain (FDTD) modeling code was developed. The integrated tool starts with the desired device geometry and an initial guess of the PnP mask parameters. It then simulates the interference pattern and filters to reveal the expected photoresist burn image. Finally, it evaluates against the desired device. An integrated optimizer makes improvements to the mask parameters and cycles the simulation again. Using a silicon-inversion method to infiltrate PnP structures, a photonic crystal with a bandgap in the near infrared (900-1200 nm) has been fabricated in collaboration with the University of Illinois, Urbana-Champaign.

Aperiodic 3D nanostructures with Penrose quasicrystal patterns have been fabricated. Quasicrystals (high short-term order and non-repetitive long-term order) are applicable for photonics and electronics as they may possess a complete bandgap. An scanning electron microscope (SEM) image of the quasicrystal-patterned photopolymer, and the FDTD simulations are shown in Figure 2. Pattern recognition software was used to make comparisons of the modeled structures to confocal images of the exposed photopolymer (green insets) and 3D nanostructures, indicating a high level of accuracy (match >80%).

The PnP fabrication method can produce 3D nanostructures over large areas (mm^2) using a simple optic and a single cycle of lithography. Creation of an accurate and predictive model allows for true design of the periodic or aperiodic 3D nanostructures having the desired optical, physical, and structural properties. Surface modification and thin film deposition onto the 3D nanostructures allows for modification of the material and chemical properties of the structures. The flexibility, ease, and cost-effectiveness of the PnP method enables fabrication of 3D nanostructures on soft or curved surfaces, creation of nanocomposite and smart materials, manufacture of structures with high surface area for chemical sensors or chemical storage, and production of nano-scale patterned surfaces/structures for studies of cell growth mechanisms and controlled-release drug delivery.

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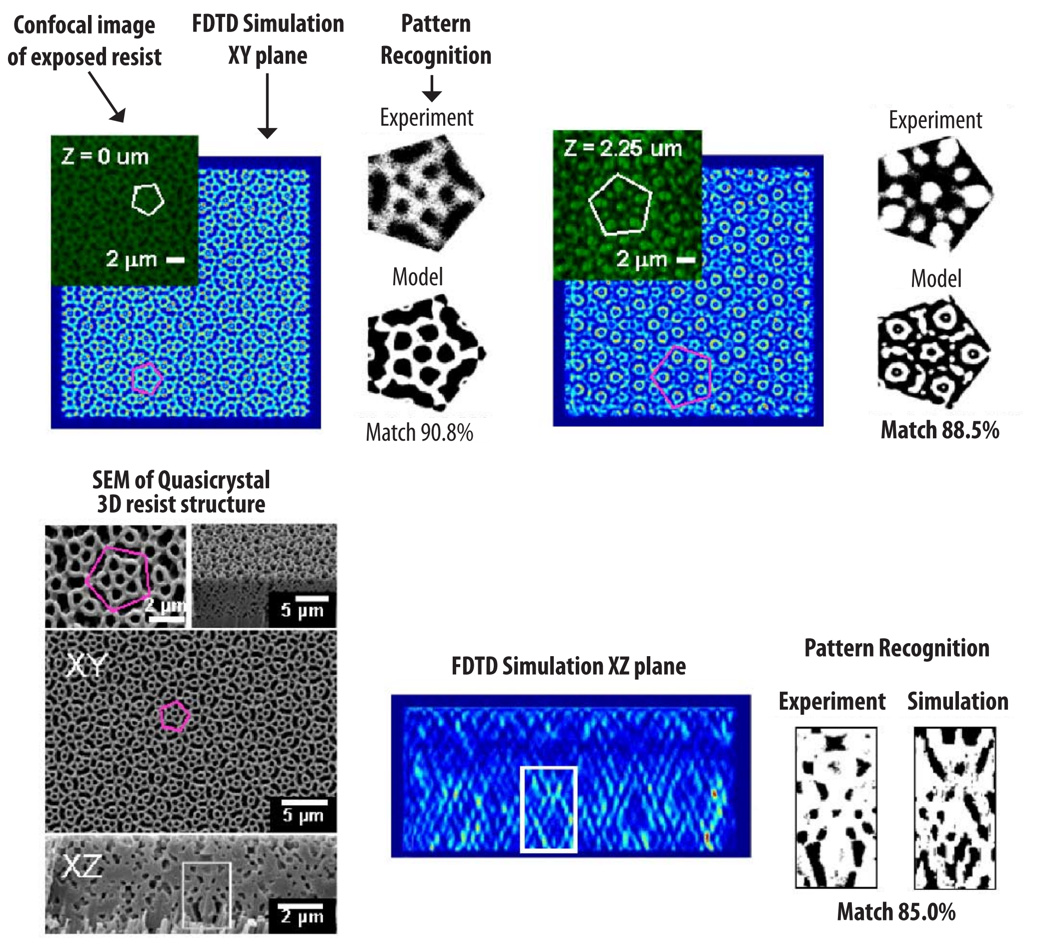

Figure 2: Comparison of SEM images (lower left) of a Penrose quasicrystal photoresist structure to FDTD-modeled resist structure in the rotational X-Y plane (blue upper left) and translational X-Z plane (blue, lower right), showing retention of 5-fold rotational symmetry in XY, and an absence of symmetry in XZ, characteristic of a quasicrystal. Also shown is a comparison to optical image (green) of exposed (but not developed) photoresist at different distances Z down from the surface. Quantitative comparison by pattern recognition methods are shown (black/white) to the right of the modeled images.

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National Nuclear Security Administration

02/2009

Solution-Templated Nano-Architectures for Ultracapacitors

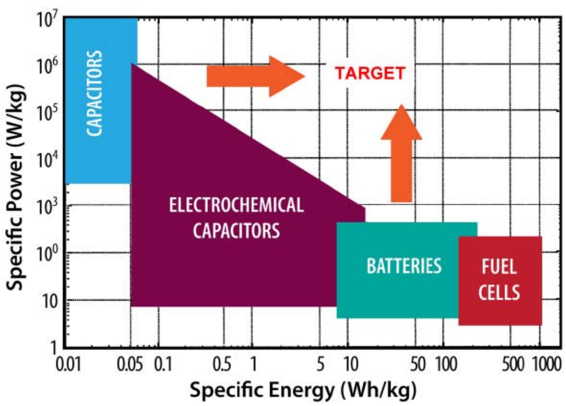

Figure 1: A Rangone plot showing energy and power characteristics of energy storage devices and future target.

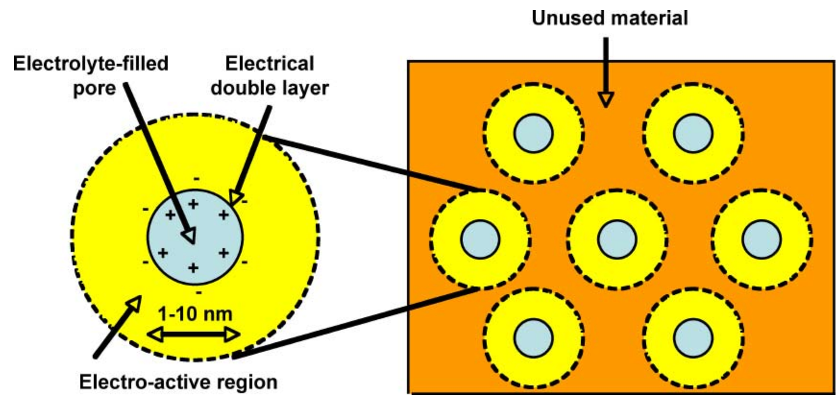

Figure 2: A schematic showing how ultracapacitors work. Electrons and counter-ions flow into and out of electroactive materials from the electrolyte. Maximum performance is achieved when all material is sufficiently close to electrolyte interfaces to be accessed.

Materials utilizing both electrochemically-active oxides and conductive polymers are promising candidates for increasing energy storage

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Electrical energy storage is becoming increasingly important to a broad spectrum of critical technologies, ranging from the electrical power grid and electric vehicles to microsystems for both commercial and defense applications. In all of these applications, the drive is to increase both energy densities (related to the charge stored per unit volume), and power densities (related to how rapidly the charge can be stored and released), as depicted in Figure 1. Ultracapacitors are unique electrical energy storage devices that can simultaneously achieve the high energy densities associated with batteries and the high switching speeds and power densities associated with capacitors within a single material. By using simple and inexpensive solution-based processing methods, Sandia researchers are now exploring ways to maximize ultracapacitor performance by producing nano-architectures utilizing both electrochemically-active oxides and conductive polymers.

To achieve the highest levels of performance, materials in ultracapacitors must be: 1) electrochemically active (capable of being oxidized and reduced under an applied voltage), 2) capable of conducting both electrons and charge-compensating counter-ions (such as protons or sodium ions), and 3) organized within a high surface area architecture to maximize contact with electrolyte solutions and minimize transport distances for electrons and ions. These ideas are shown schematically in Figure 2. Sandia is exploring a wide range of solution-based schemes in which structural elements that are of nanometer dimensions (tens of atoms thick) are used as templates for the growth of electroactive materials (Figure 3). In some instances, arrays of organic surfactants serve as templates for creating nano-architectures in electroactive oxides, while in other instances, high surface area oxides are used as templates for the polymerization of conductive polymers. In mixtures containing both active oxides and conductive polymers,

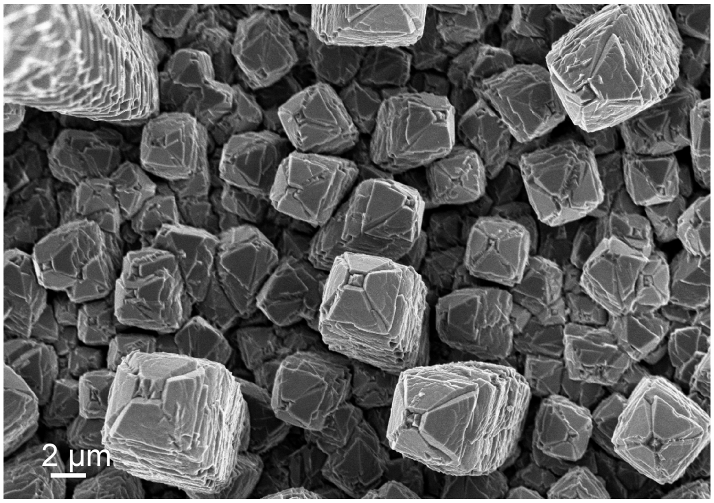
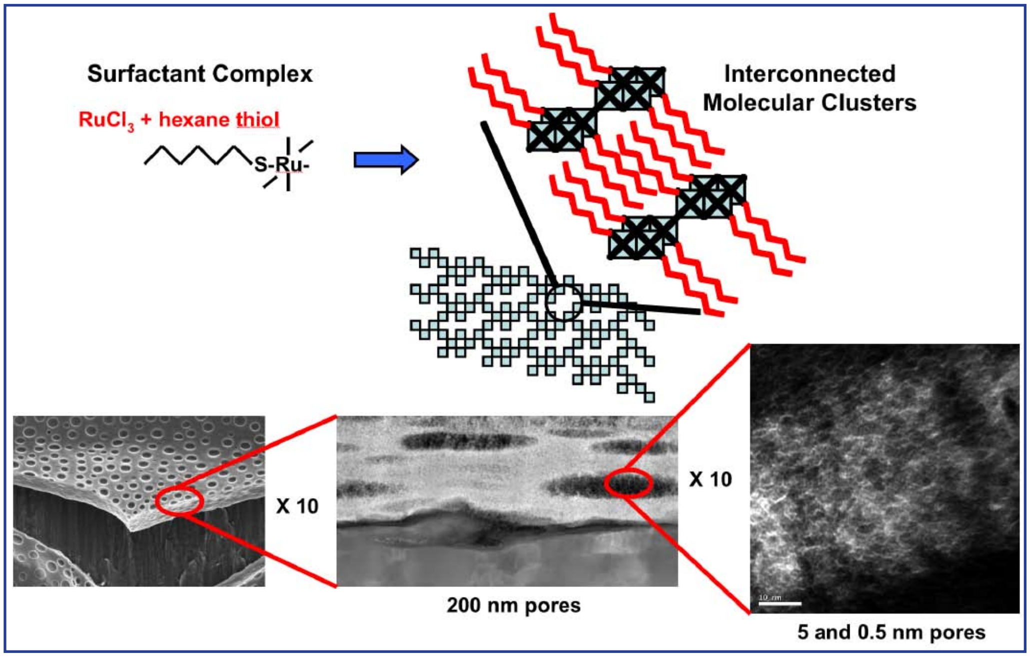


Figure 3: An electron micrograph of hydrothermal $MnTiO_x$ grown at Sandia. Here, clay-like nano-layers within each pillar provide electrolyte access rather than pores.

each material in the nanostructure can contribute to the overall performance. One element may provide conductive pathways for electrons, while another material provides conductive pathways for ions.

A specific example showing the benefits of solution-prepared nanostructures is provided by the use of surfactants to organize the formation of electrochemically active ruthenium oxide (Fig. 4). Sulfur groups in the surfactants bond to the dissolved ruthenium species used to produce thin films via spin coating. The surfactant sterically blocks sites that would normally be available for the formation of an extended oxide. On heating, the surfactant decomposes, leaving behind a structure consisting of interconnected molecular clusters having sub-nanometer dimensions. Electrochemical measurements show that this structure has over three times the capacitance and power density of bulk ruthenium oxide. This is because: 1) all ruthenium atoms are within a few atomic dimensions of the electrolyte solution, minimizing transport distances, and 2) the clusters retain high hydroxyl group concentrations, providing for enhanced proton conductivity. Work is now progressing to systems containing conductive polymers with redox potentials, energy densities, and power densities that can be selectively tuned to match a broad range of energy storage applications. Early results indicate that it should be possible to achieve performance enhancements using materials that are substantially cheaper and easier to make than ruthenium oxide. Sandia is also starting to explore how similar templated techniques could be used to create nano-architectures that are optimized for anodes, cathodes, and separators for batteries and other energy storage systems.

Figure 4: (Top) - Ruthenium-surfactant complexes (left) react with each other to form interconnected molecular clusters of ruthenium oxide. (Bottom) - Electron micrographs show that the resulting films exhibit hierarchical porosity to optimize electrolyte access and minimize transport distances. Large pores are bubbles forms via template decomposition, while small pores are defined by the molecular clusters of RuO_2.



Effect of Interfacial Polymer Morphology on Solar Cell Performance

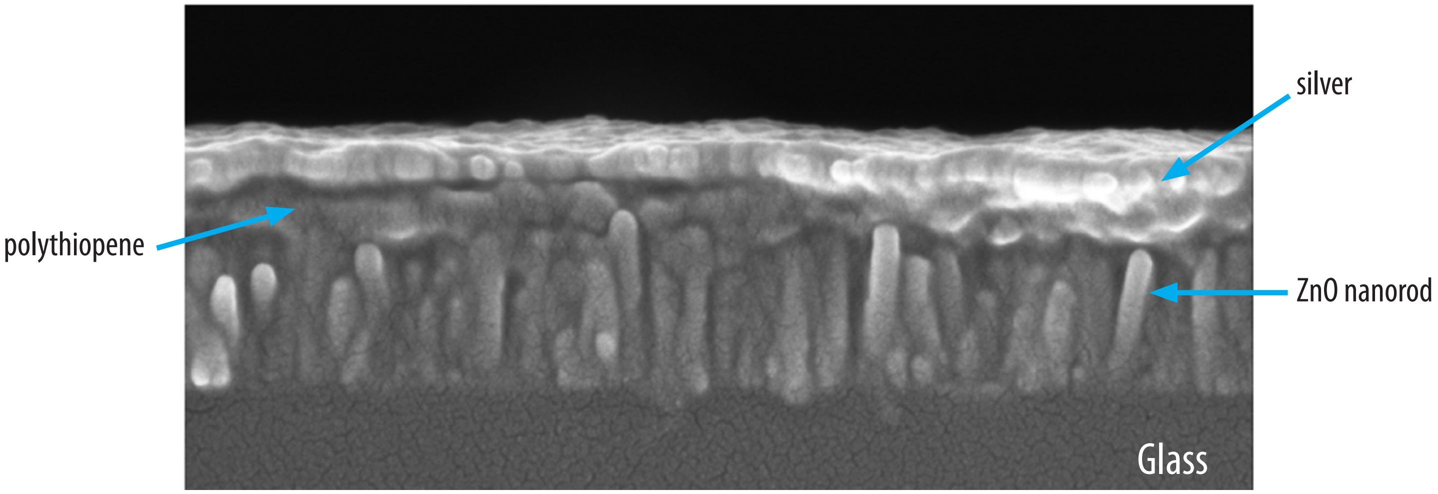


Figure 1: Cross-sectional scanning electron microscopy of a polythiophene-ZnO nanorod hybrid solar cell.

Organic-inorganic hybrid photovoltaics are studied by Sandia team

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The proliferation of new, high technology gadgets that make our life more convenient and enjoyable require evermore portable and reliable energy sources. Solar cells using organic photovoltaic (OPV) technology, with its light weight, flexibility, and inexpensive manufacturing process, appear to be uniquely suited to meet these new requirements. A subset of OPVs, called hybrid photovoltaics, uses organic polymers to generate carriers (electrons and holes) and inorganic metal oxide semiconductors as the electron acceptor material. The advantages of hybrid photovoltaics over purely organic counterparts include environmental stability, better electron transport, and the ability to optimize interfacial properties.

Sandia researchers, in collaboration with the National Renewable Energy Laboratory, have focused on understanding and optimizing hybrid solar cells that utilize nanostructured zinc oxide (ZnO) as the electron acceptor. The research challenges to making such solar cells practical are the ability to achieve highly dense oxide nanostructures (Figure 1), to infiltrate organic conjugated polymers into the ZnO nanostructures while maintaining polymer crystallinity, and to optimize the charge transfer process at the polymer-oxide heterojunctions. Synthesizing ZnO nanostructures from solution at low temperature is a particular expertise of the Sandia team. However, it was realized that the normally crystalline organic polythiophene forms a thin amorphous layer at the ZnO interface. This morphological change in the organic material is detrimental to solar cell performance as it shortens exciton diffusion length, reduces overlap with the solar spectrum, and degrades hole transport.

To understand and overcome this problem, Sandia modified the ZnO-polythiophene interface with a self-assembled monolayer of alkanethiols. These are long hydrocarbon chains that form chemical bonds with the ZnO but interact only weakly with the polythiophene. Since alkanethiols are also insulating molecules that form a barrier for electron transfer from polythiophene to ZnO, it was surprising when a higher than expected photocurrent was observed in these modified solar cells (Figure 2). Further research, using grazing-incidence X-ray diffraction (at the Stanford synchrotron) and femtosecond transient spectroscopy (at the Sandia-Los Alamos Center for Integrated Nanotechnologies in collaboration with Los Alamos National Laboratory), revealed that the alkanethiol layer indeed restored the crystallinity of the interfacial polymer (Figure 3). The crystalline form of the polymer greatly reduced the carrier recombination rate. Thus, despite the insulating alkanethiol layer between the polymer and the ZnO, the overall efficiency of the hybrid solar cell was improved.

These results highlight the importance of understanding nanometer-scale details of the interface, as nanoscale behavior has dramatic impact on the macroscopic performance of innovative new devices.

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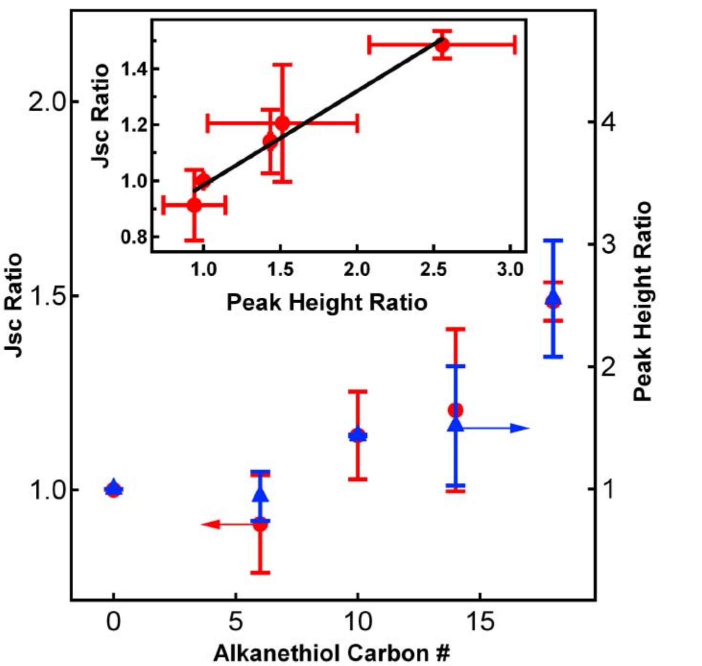


Figure 2: Increases in photocurrent (left axis, red circles) and polymer interchain order (right axis, blue triangles) as a function of the chain length of the interfacial organic modifier. Inset: the two increases are clearly correlated.

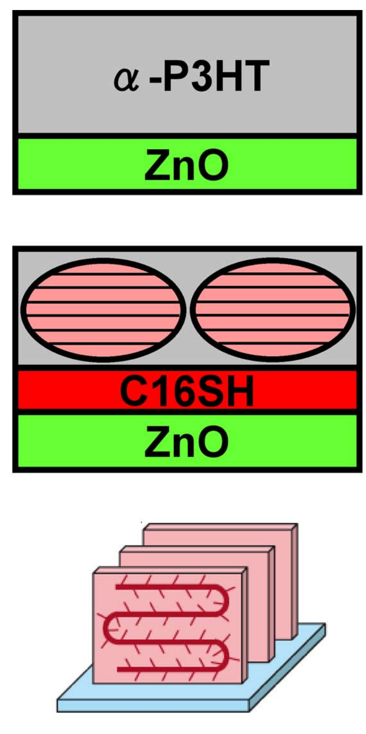
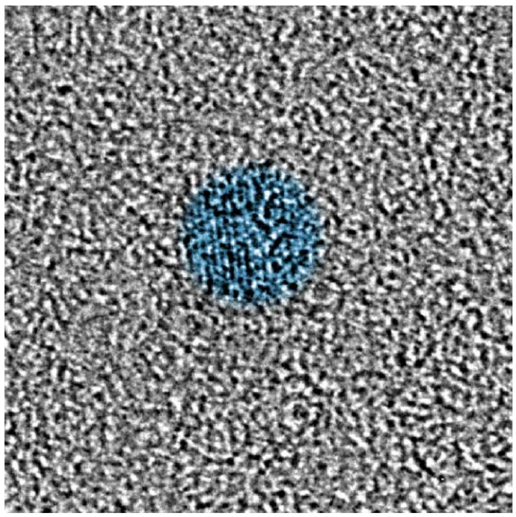


Figure 3: Schematics of polymer morphology change due to interfacial modification with a C_{16} alkane thiol at the ZnO interface. The amorphous polythiophene polymer(gray) becomes crystalline (pink areas) when the alkane thiol (red) is present. Detailed view of the crystalline regions (pink areas) is shown at bottom. (Y. Kim, et al. Nature Mater. 2006, 5, 197)

Materials Science and Technology
Nanotechnology

Tuning the Properties of Magnetic Nanoparticles Through Surfactant Design



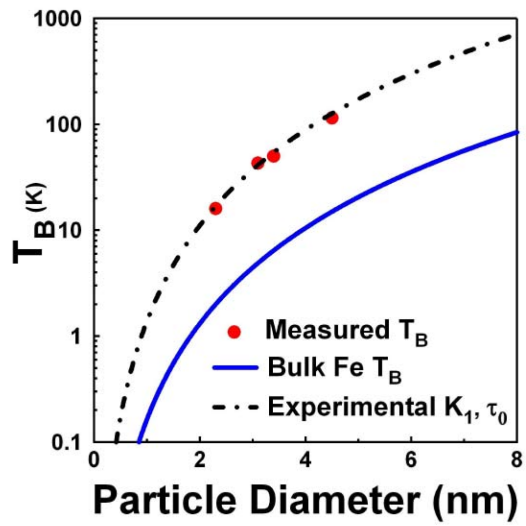


Figure 1: (Left) A transmission electron micrograph of a single 3 nm iron nanoparticle (colorized for enhanced visibility), with no detectible oxide, and complete lattice fringes demonstrating the single crystal nature of the particle.

Figure 2: (Right) Plot of the measured blocking temperature for a series of different sizes of iron nanoparticles, fitted by an Arrhenius function (dash-dotted line) using the measured magnetic anisotropy (K1) for the nanoparticles. A curve of the values expected for bulk iron is shown in solid blue.

The control of magnetic properties of nanoparticles has been a long-time goal for science and industry

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Magnetic phenomena on the nanoscale are of growing interest for both scientific and technological reasons. For example, much of our modern information storage is based upon magnetism, and there is a continuous need for higher density storage and therefore smaller structures. The basics of nanomagnetism have been understood for decades for simple, well-behaved systems. Unfortunately, the only nanomagnets that behave well are those that are isolated both from each other and from a strongly interacting matrix material. Classical examples are particles suspended in a vacuum or inert carrier gas. For technological applications, it is critical for nanomaterials to be imbedded in some matrix material that will invariably alter their magnetic properties. Sandia's goal in this research is to understand, at a fundamental scientific level, how these matrix interactions alter the magnetism of nanoparticles. This fundamental knowledge will then enable the use of these materials in a variety of important technologies.

Since surfactants are a critical component in the nanoparticle synthesis, Sandia is examining how the choice of surfactants modifies the magnetic properties of nanoparticles. A system of un-oxidized iron nanoparticles was chosen as a model because of two important properties: it is both highly magnetic and extremely reactive. Thus the effect of chemical interactions between the surfactants and the nanoparticle surfaces should be easily detected.

A recently developed synthesis that utilizes beta-diketone-based surfactants has been shown to produce oxide-free, single crystal, iron nanoparticles (see Figure 1). These nanoparticles have a much higher effective magnetic anisotropy than would be expected for bulk iron, making them much "harder" magnets. Data that demonstrate this are shown in Figure 2, where the blocking temperatures of a series of iron particles of varying diameter are plotted. (The blocking temperature is the temperature below which magnetic nanoparticles behave as permanent magnets, and above which their magnetic moment freely reorients.) Based on a calculation using the bulk properties of iron, the expected blocking temperature is below 1K for the smallest particles shown. However, the data indicates that for all the particles tested, the blocking temperature is more than ten times the value predicted.

In contrast, performing the same synthesis using a more conventional polyether-based surfactant produces particles with bulk-like magnetic properties. Thus, by merely changing the organic matrix surrounding an iron nanoparticle, the magnetic hardness of the material can be altered by more than an order of magnitude. It appears that the extremely high anisotropy is a material property induced by the beta-diketone surfactant used. This hypothesis has been confirmed to the extent that unusual crystalline structure in these particles has observed with high energy X-ray diffraction. Developing an atomic level model of the structure of these particles and understanding how to systematically control it is the subject of ongoing research.

Because of the immense technological benefits, the control of the structure and magnetic properties of nanoparticles has long been a goal of materials science. For example, 2-5 nm magnetic particles could be used as bits for information storage if they are magnetically hard enough (have a high enough anisotropy). On the other hand, highly-efficient magnetic refrigeration requires lower anisotropy to maximize the magnetocaloric effect. Thus tuning the properties of the finite number of magnetic materials by varying surfactants could provide many new useful materials. This work is a step in that direction as Sandia has taken a famously soft magnetic material and made it a hard magnet.

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Converting Fermions to Bosons in Electron-Hole Bilayers

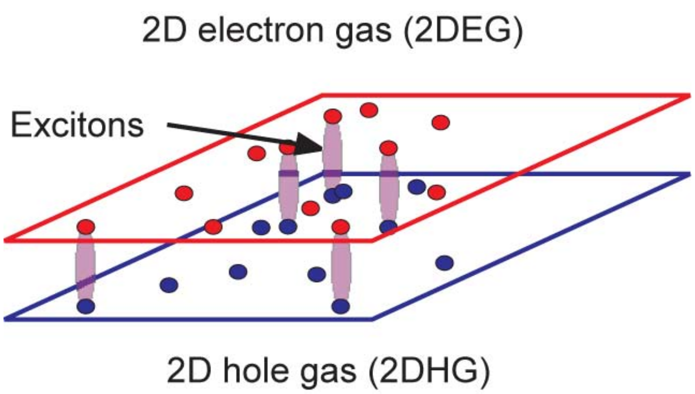

Figure 1: Excitons are present as electron and hole pairs that form across opposite layers.

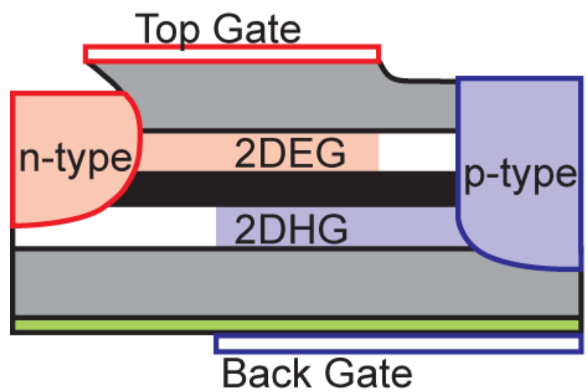

Figure 2: Schematic cross section of the undoped electron-hole bilayer sample: the conducting areas of the 2DEG (2DHG) are in red (blue), the $Al_{0.3}Ga_{0.7}As$ ($Al_{0.9}Ga_{0.1}As$) barriers are in grey (black), and a insulating SiN layer is shown in green.

Fundamental low temperature physics is made possible by Sandia's expertise in heterostructure growth and device fabrication

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In quantum mechanics, a particle is identified by a wavefunction that contains spatial and spin components. Collections of identical particles obey fundamental statistical rules that are determined by their spin state. Particles with half-integer spins (e.g., electrons) are fermions, and particles with integer spins (e.g., photons) are bosons. Electronic, thermal and other properties are strongly impacted by the these statistics. For example, fermions must obey the Pauli exclusion principal that doesn't allow any two fermions to occupy the same quantum state. Bosons, on the other hand, can occupy exactly the same state, and at very low temperatures they collapse into a single quantum state called a Bose-Einstein condensate (BEC). Interestingly, when two fermions couple together, they look like a boson. One case where this occurs is when an electron and hole pair up in a semiconductor and form an exciton (Figure 1). Experiments at Sandia are trying to identify the transition from electrons and holes acting like fermions to the exciton acting like a boson.

Creating the appropriate electron and hole systems is extremely challenging. For BEC to occur, the electrons and holes need to be confined to two dimensions and be spatially separated into a bilayer. Sandia's expertise in growing high quality GaAs heterostructures and performing advanced semiconductor processing is critical to the success of this project. A cross section of a structure is shown in Figure 2. The primary measurement in these systems is a four-wire resistance measurement at very low temperature.
For the typical resistance measurement in electronic materials, current is driven between two contacts and the voltage is measured between two different contacts. In the Sandia bilayers, current is driven in the electron layer and voltage is measured in a *different* layer, as shown in Figure 3. This configuration is called Coulomb drag, and the resistivity has units of Ω/☐ where ☐ represents the length divided by the width. For weakly coupled electrons and holes, the Coulomb drag measurement is dominated by electron-hole scattering, and vanishes as the temperature is

reduced. When excitons form, the electronic coupling between the layers is much larger, and the drag signal is expected to increase. In fact, the drag is predicted to diverge when Bose-Einstein condensation occurs.

In Figure 4, the drag resistance (ρ_{DRAG}) for three devices is shown for electron (n) and hole (p) densities $n = p = 8 \times 10^{10}\ cm^{-2}$. Each has a different barrier thickness between the electron and hole conducting layers (see Figure 2). The drag for the wider barrier sample (green, 30 nm barrier) is quadratic with temperature. The two narrow barrier devices (blue and red, 20 nm barrier) are initially quadratic, but below the temperature of 0.5 K a significant deviation develops. Here the drag reaches a minimum, and for lower temperatures there is a pronounced *upturn* of ρ_{DRAG} where it *increases with decreasing temperature*. The increase in drag indicates the development of a strong coupling between the electron and hole layers. While there is not enough evidence to conclude that Bose-Einstein condensation has occurred, we believe the increase in drag is due to the formation of excitons in the system. Thus, the next step is to fabricate and study electron-hole bilayer structures with thinner barriers and at lower temperatures . Another step is to broaden the transport techniques to include counter-flow where currents are flowing in opposite directions in each layer. The counter-flow measurement is expected to be sensitive to the superfluid component of an exciton condensate.

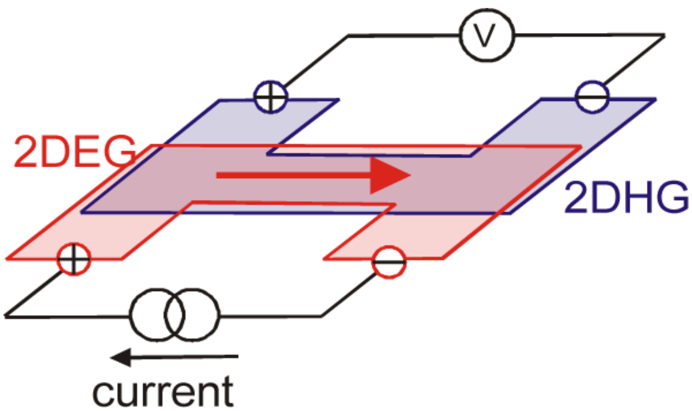

Figure 3: Coulomb drag measurement where current flows in electron (2DEG) layer while voltage is measured in the hole (2DHG) layer.

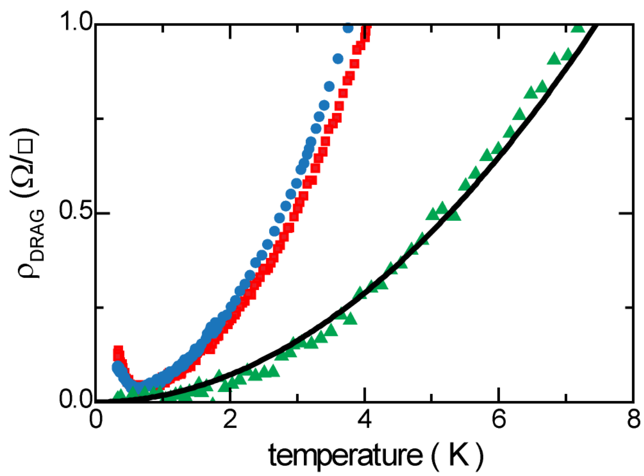

Figure 4: Drag resistivity at n = p = 8 x 10^{10} cm^{-2} for three devices. Sample A, 30 nm barrier, (green triangles), Sample B, 20 nm barrier, (red squares), and Sample C, 20 nm barrier, (blue circles). The line is a T^2 best fit for the electron hole bilayer with a 30 nm barrier.

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Materials Science and Technology
Nanoscience

Interfaces in Thermoelectric Materials

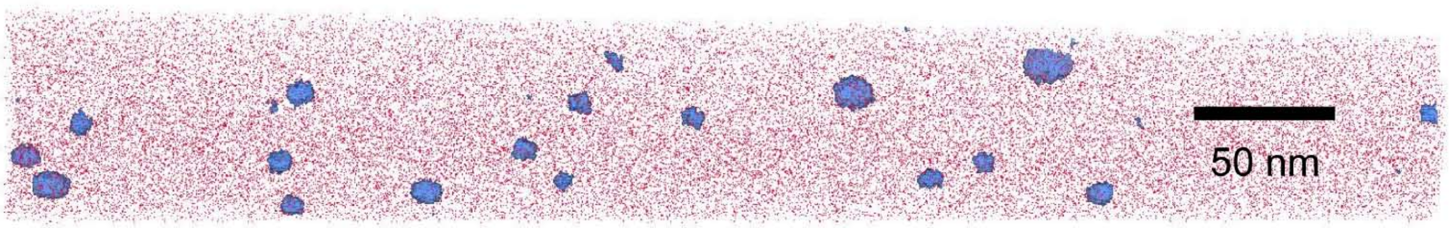

Figure 1: Using advanced microscopy techniques, such as atom probe tomography, Sandia researchers are investigating the mechanisms of nanostructure formation in thermoelectric materials. This example shows the three-dimensional distribution of embedded nanoscale Ag_2Te precipitates in PbTe.

Experiment and theory are providing new insights in nanostructured thermoelectric alloys

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Thermoelectric materials have many applications in the conversion of thermal energy to electrical power and in solid-state cooling. Although thermoelectric devices have found many specialized applications where their high reliability, lack of moving parts, and ability to be scaled to small sizes provide key advantages, the energy conversion efficiencies of these devices remains generally poor. For more wide-spread use of thermoelectrics, the material and device efficiencies will need to be improved dramatically. To address this need, Sandia is building an effort that bridges synthesis, characterization, and thermoelectric measurements, as well as theory and modeling, to harness the potential of nanostructured bulk materials for thermoelectricity.

The energy conversion efficiency of a material is characterized by the thermoelectric figure-of-merit:

$$zT = \frac{\alpha^2 T}{\rho\kappa}$$

Approaches to improve thermoelectric conversion efficiency are driven by the need to maximize the Seebeck coefficient, α, and to balance the competing requirements of low electrical resistivity, ρ, and low thermal conductivity, κ. Interfaces affect each of these properties and can have profound effects when present at the high densities typical of nanomaterials. Recent advances have shown that zT can be enhanced in nanoscale systems by taking advantage of phonon scattering at interfaces to reduce thermal conductivity and quantum confinement and carrier scattering effects to enhance the power factor, α^2/ρ.

Sandia is investigating the formation and stability of interfaces in thermoelectric nanomaterials and how these interfaces control thermal and electronic transport. Advanced microscopic tools, such as atom probe tomography (Figure 1) and electron microscopy, are being used to better understand how embedded nanostructures can form in bulk thermoelectric alloys. For instance, recent work on $AgSbTe_2$, a high-performance thermoelectric material, has clarified the complex phase transformation mechanisms that occur in this system. This material forms fine-scale precipitates of silver telluride (Ag_2Te), which is monoclinic at room temperature. By establishing how these precipitates are oriented (Figure 2), Sandia has shown that the Te-sublattice remains aligned in both the matrix and precipitate phase. Because the monoclinic and high-temperature cubic phases of Ag_2Te differ by only small, local distortions of the crystal lattice, this result suggests a facile transformation path for the Ag_2Te precipitation, requiring only the clustering of excess silver. Given similar observations in PbTe-based materials, it appears that this mechanism is generic to rock-salt structured tellurides.

The experimental work is supported and guided by theory and modeling, where Sandia is developing models to better explain how nanostructures improve thermoelectric properties. Recently, it was shown that nanoscale metallic precipitates can enhance the thermoelectric properties of bulk semiconductors. The idea behind this work is that the presence of a potential well or barrier near the nanoparticle surface causes low-energy electrons to be strongly scattered while allowing high-energy electrons to be unaffected (Figure 3). Thus the nanoparticle/matrix interface serves as an energy filter for electrons. This filtering effect increases the voltage that is generated across a bulk thermoelectric material when a temperature gradient is applied across it (the so-called Seebeck effect). The nanoparticles also play a dual role: because the sound velocity is different in the nanoparticles and the matrix, heat transport through phonons is reduced. This effect, when combined with the electron energy filtering effect, can lead to large enhancement in the energy conversion efficiency.

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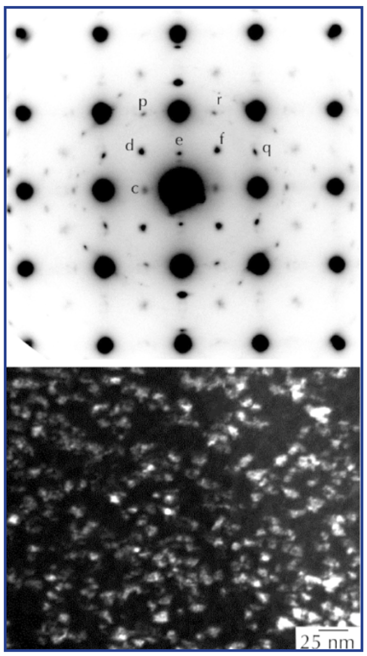

Figure 2: Electron diffraction (top) and dark-field transmission electron micrograph (bottom) showing nanoscale Ag_2Te precipitates in a matrix of thermoelectric $AgSbTe_2$. The orientation results from alignment of the Te sublattices in the two phases.

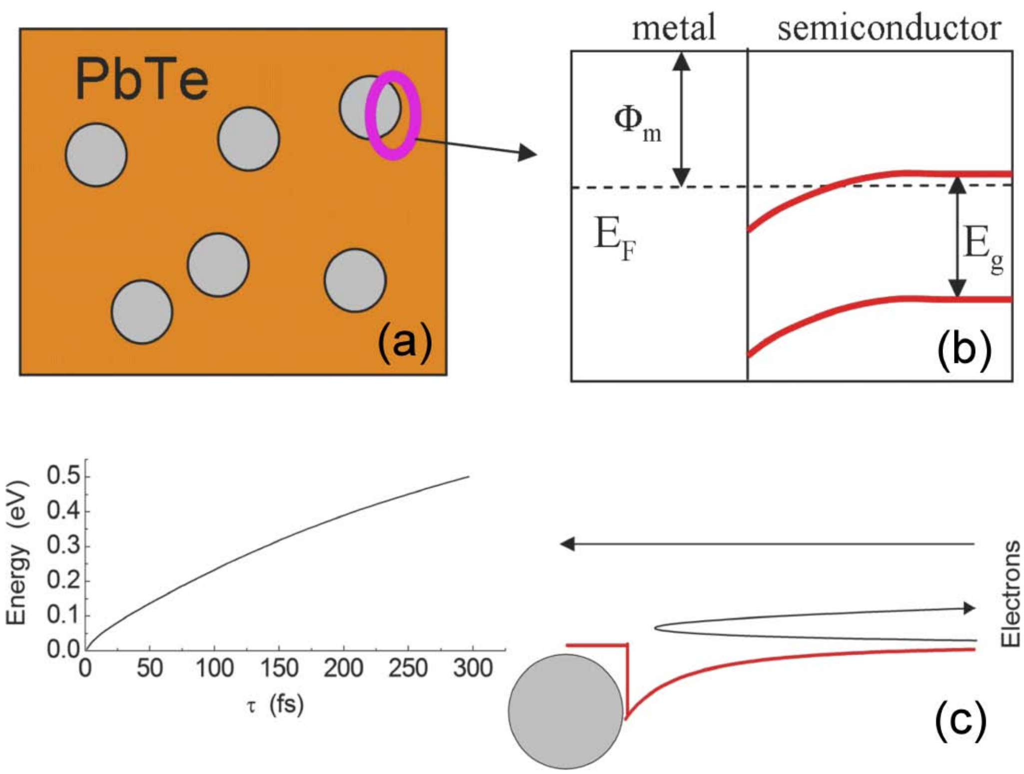

Figure 3: *Panel (a)* Schematic of semiconductor host with metallic nanoinclusions. *Panel (b)* shows an example of the calculated potential and the energy diagram for PbTe with Pb nanoinclusions of radius 1.5 nm. E_F is the Fermi level, E_g is the semiconductor bandgap and Φ_m is the metal work function. *Panel (c)* illustrates the concept of energy filtering: low energy electrons scatter strongly with the potential, but high energy electrons are unaffected. The calculated electronic relaxation time for the potential of panel (b) is also shown.

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Platinum Nanostructures for Enhanced Catalysis

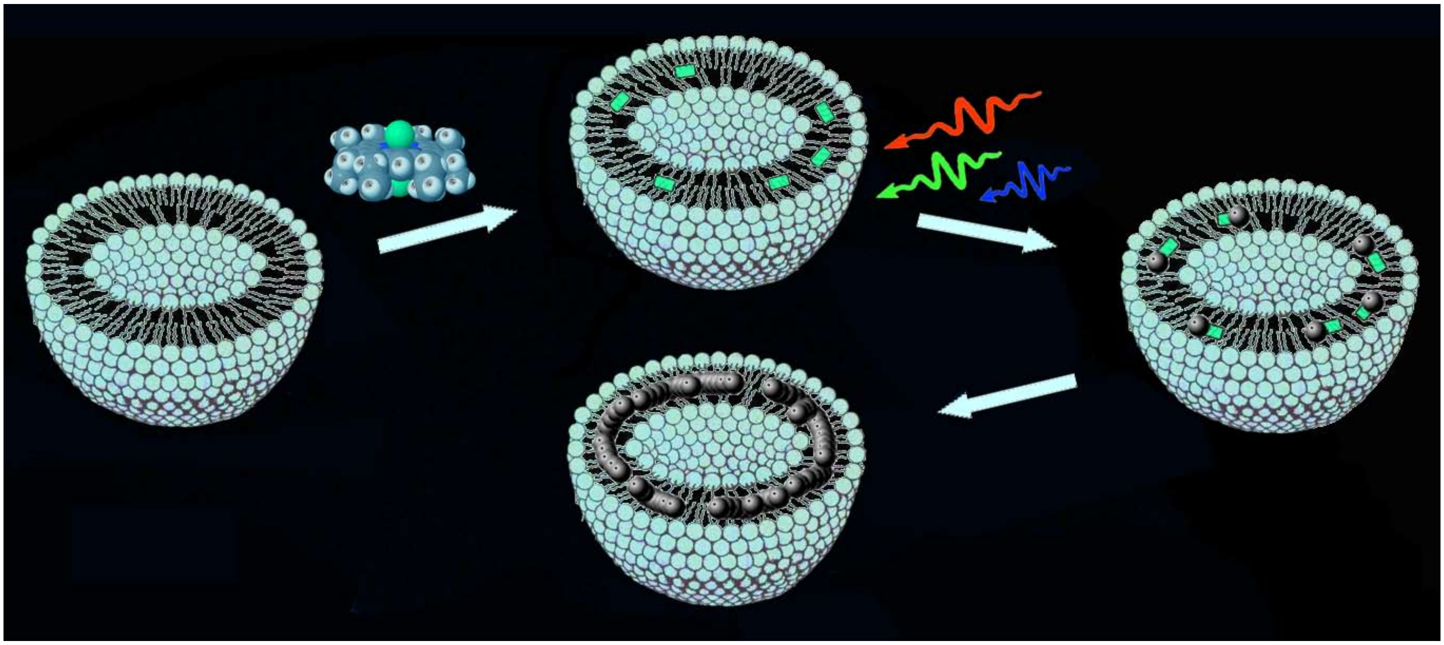

Figure 1: Schematic of how platinum nanostructures are formed. In this case, spherical surfactant liposomes, which incorporate photoactive porphyrins, template the reduction of Pt complexes into platinum metal at the porphyrin sites when exposed to light. The resulting Pt structures are shown in Fig. 2.

Complex platinum structures offer promise as improved catalysts in hydrogen fuel cells

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One of the promising renewable energy technologies today is the hydrogen-powered fuel cell. A key challenge for fuel cells in their ability to be a practical and cost-effective solution to meet energy needs is for more durable, efficient, and inexpensive electrocatalysts. Since it is well-known that platinum is the best substrate for catalytic reactivity, it is paramount that the rare and expensive material be used as sparingly and efficiently as possible. Sandia has developed an innovative approach for producing platinum catalysts at the nanoscale that offers much greater control over the shape, size, porosity, composition, stability, and other functional properties than those achieved by previous methodologies. Due to the high surface area and durability of the nanostructures, the process is expected to reduce platinum usage not only in fuel cells, but in other applications in the renewable energy sector as well.

The platinum nanostructures are produced by controlling the dendritic metal growth that, under certain circumstances, occurs during the chemical reduction of aqueous platinum molecular complexes (Fig. 1). Dendritic growth produces branching metal arms that are approximately 3 nm in width with spaces between the branches of about 1 nm. Control over the structure is through a combination of a photoactive seeding method and the use of soft or hard nanostructured templates. Seeding is initiated by light absorption at porphyrins dispersed in the templates, followed by localized metal formation at these sites. Soft templates include surfactant assemblies such as liposomes (Figs., 1, 2), liposomal aggregates (Fig. 3), bicelles (Fig. 4), and worm-like micellar networks (Fig. 5); whereas, hard templates include inorganic or organic microspheres.

The electron micrographs in Figures 2-5 clearly demonstrate how the size and shape of platinum structures can be manipulated at the nanoscale. Of particular note are structures composed of dendritic "nanosheets," such as the spherical dendrites shown in Fig 3. Remarkably, these structures can be transformed into "holey sheets" that exhibit enhanced structural durability under thermal, catalytic, and electrocatalytic reaction conditions. The structural durability comes from a resistance to ripening, a process by which small structural features become larger (e.g., during fuel cell operation) resulting in decreased active surface area. These ripening-resistant platinum nanostructures thus preserve the high surface area and catalytic activity.

Competing technologies mainly consist of platinum nanoparticles dispersed on conducting carbon substrates. Shaped platinum nanomaterials offer enhanced structural durability, specific activity, and long range conductivity because of their extended metal structures. They also have advantages in the materials processing and fabrication of fuel cell electrodes. The Sandia technology is described and documented in ten patents and patent applications that have recently been licensed by Sandia to Compass Metals, Inc. for commercialization in the area of fuel cells. Compass Metals is also supporting a cooperative research and development agreement (CRADA) with Sandia to refine and improve the large scale synthesis of these novel catalytic materials for commercial use, to develop more advanced catalysts, and to investigate methods for their optimum use in fuel cells.

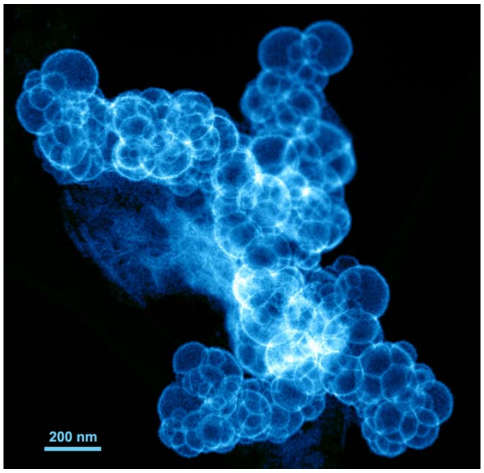

Figure 2: Pt nanocages produced by the method illustrated in Fig. 1. Each spherical cage is composed of many joined nanodendrites grown inside the bilayer of a unilamellar liposome.

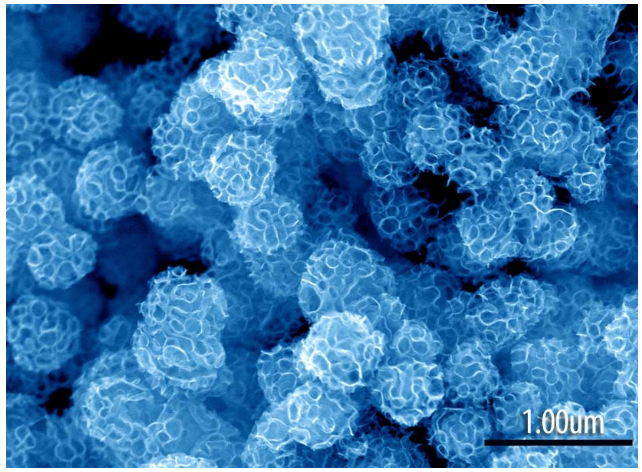

Figure 3: Platinum nanospheres composed of convoluted dendritic nanosheets templated by liposomal aggregates. The scale bar is 1 micron.

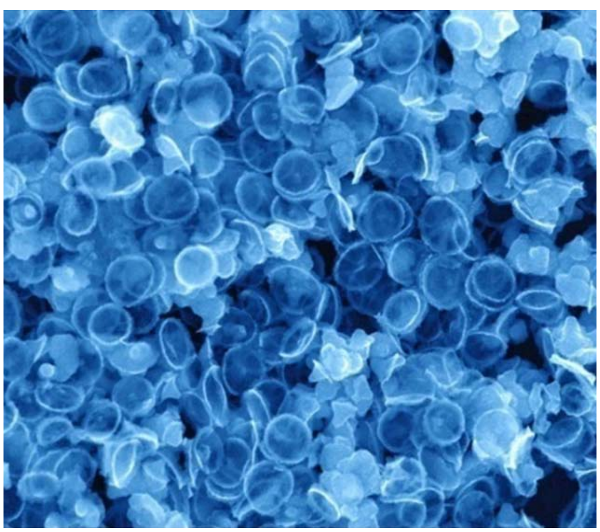

Figure 4: 300-nm platinum nanodisks templated by surfactant bicellar disks.

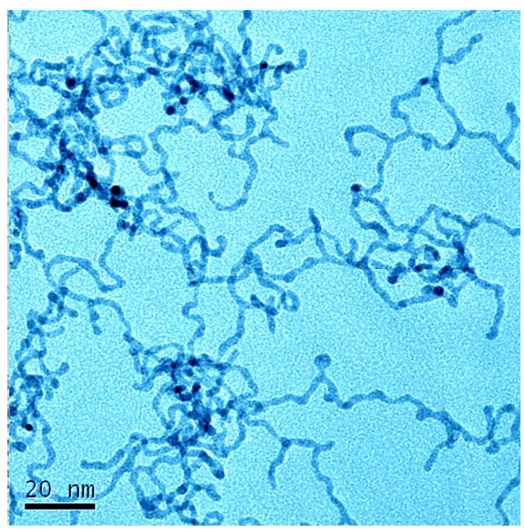

Figure 5: 2-nm diameter platinum nanowire networks templated by worm-like micellar networks.

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Microscale Thermoacoustic Engines

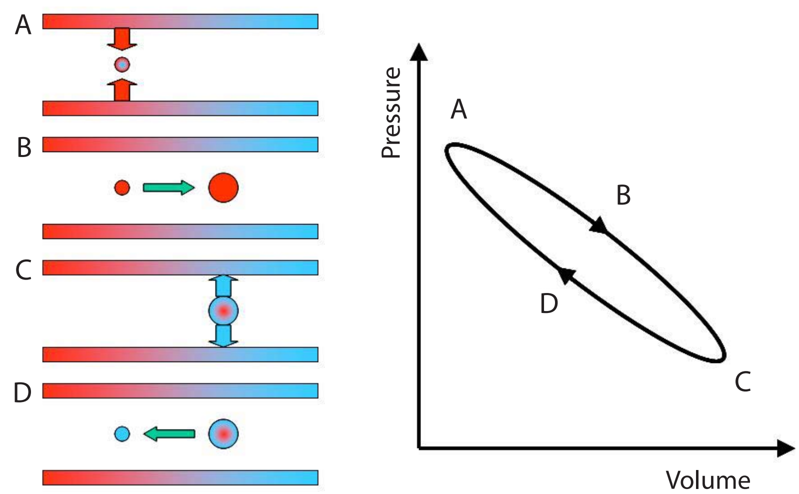

Figure 1: The principles of thermoacoustic operation. At (A), heat is added to a parcel of air, at the same time that it is being compressed by a sound wave. At (B), the heated parcel moves from hotter to cooler regions of the stack, expanding as it goes. At (C), the expanded parcel rejects heat to the walls of the stack, but continues to expand. At (D), the parcel moves towards the hot end of the stack, compressing as it goes.

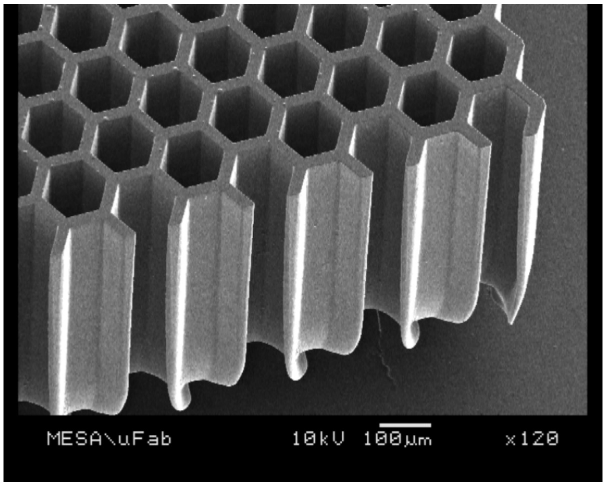

Figure 2: Scanning electron micrograph of a microscale thermoacoustic engine stack. The tubes resonate like a pipe organ, launching acoustic energy that can be later converted into electrical power. It is manufactured lithographically from a photosensitive polymer. The walls of the tubes are only 15 µm across, and the stack stands a little over 1 mm tall.

Heat engines harvest electrical power from low grade heat that is normally lost

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For every joule of energy that is converted into useful work, several joules of energy are lost through the generation of heat. Since much of this heat is localized and in close proximity to a much cooler environment, temperature gradients are usually present when work is performed. In order to reclaim some of this wasted energy, efforts are being made to develop "heat engines," mechanical devices that extract work from heat gradients. By miniaturizing robust heat engines, Sandia hopes to use them to power small devices.

Large scale heat engines typically work by letting a working fluid (either a liquid or a gas) absorb and reject heat in a specific order such that the pressure change that the working fluid experiences acts upon a piston or other mechanical device. However, this technology is difficult at the microscale due to the challenges of producing leak-free minature sliding seals and friction-free moving parts. Instead, in conjunction with Los Alamos National Laboratory (LANL), Sandia has developed a miniaturized thermoacoustic engine (Fig. 1), where the heat gradient sets up an acoustic resonance like the sound from a pipe organ. These engines thus have tuned pipes to launch sound waves from a collection of precisely sized tubes. By making the tubes just the right size, and having tuned volumes above and below them, the pipes produce an energetic sound wave that drives a membrane into resonance. Mechanical energy in that vibrating membrane can then be converted into electrical power.

The critical determinant of thermoacoustic engine efficiency is the accurate production of groupings of tuned pipes, known as the "engine stack." Using its microfabrication facilities, Sandia has recently demonstrated the manufacture of an efficient microscale engine stack (Fig. 2), as well as several other critical components of a small scale thermoacoustic engine. A fully assembled engine, with micro-scale crystalline silicon heat exchangers that help transfer the heat uniformly across the hot and cold sides of the engine stack, is slightly less than a quarter of an inch tall (Fig. 3).

From simulations of the performance, the Sandia-LANL team predicts that a heat gradient as little as 10 °C, and heat fluxes as low as 20 mW/cm^2, could result in 10-100 $\mu W/cm^2$ of mechanical power. Significant challenges remain prior to producing a working device, such as filling the stack with the correct working fluid, and creating a membrane that can integrally convert mechanical into electrical power. Small engines like these could make use of heat in car engines to power small sensor systems or other electronics. Other examples include using sun-warmed rocks for border security sensors, or continuously powering pressure sensors in power generating turbines, giving early warning of failures or overpressures. Whatever the application, the ability for minature engines to scavenge otherwise wasted energy and turn it back to useful power is sure to be welcome.

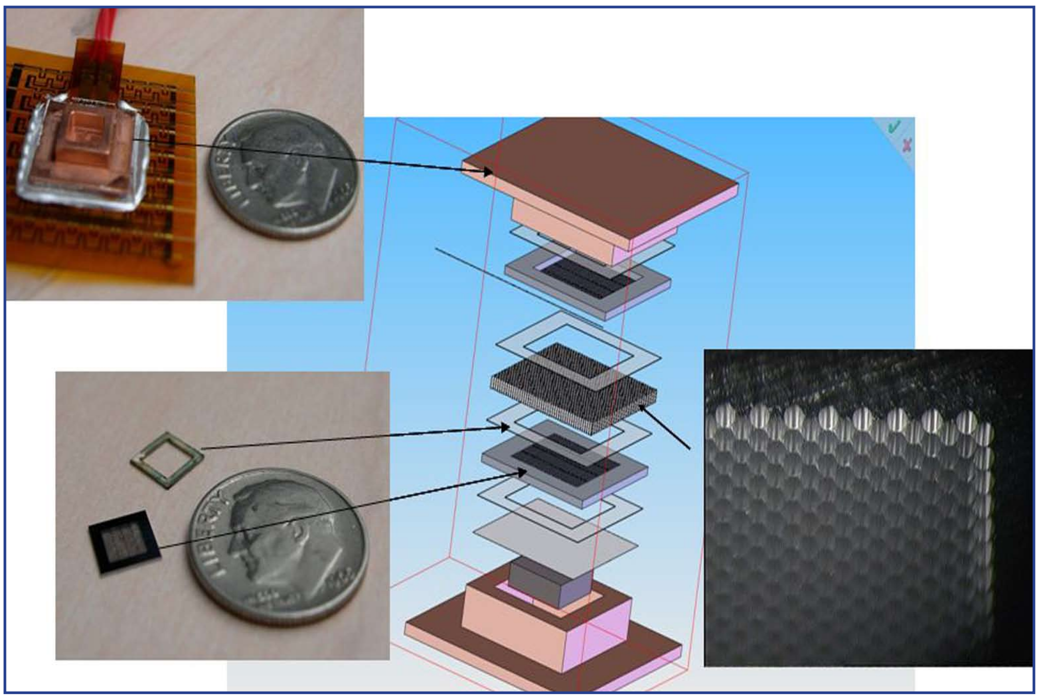

Figure 3: Assembly schematic of a microscale thermoacoustic engine, along with some of the subcomponents. The upper left figure shows a heat concentrator and heat flux monitor. The lower left shows a close up of a silicon micromachined heat exchanger and a gasket. The lower right shows an earlier version of the stack, made by using synchrotron radiation to pattern a polymer.

Miniature Flow Cytometer

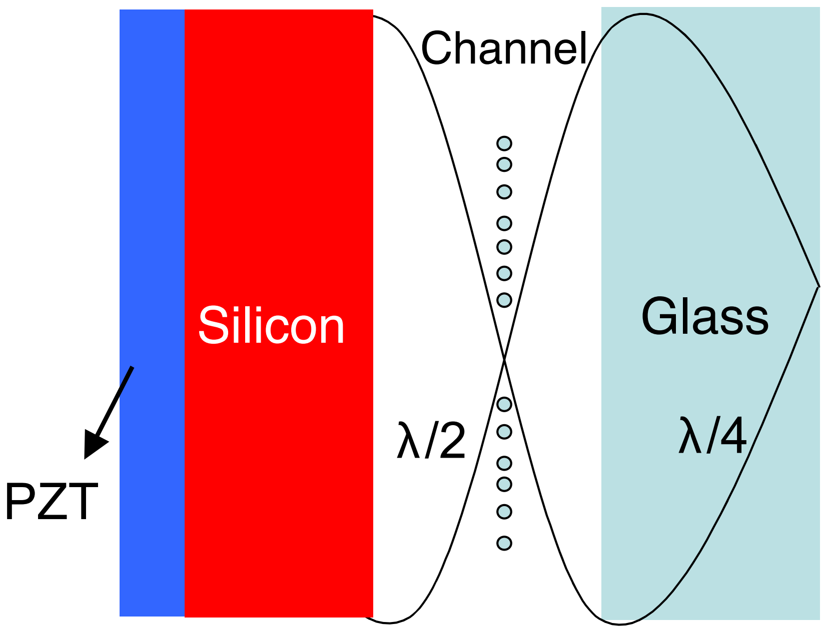

Figure 1: Schematic of the miniature flow cytometer concept, illustrating how acoustic standing waves (wavelength λ) are used to control particle position within a micromachined microchannel. When the piezoelectric acoustic transducer (PZT) is turned on, flowing beads or cells move to the center of the channel where there is an acoustic pressure node.

Acoustic focusing is used to control particle position within microchannels

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Since the 1970s, flow cytometry has been a cornerstone technology in both research and in clinical diagnostics, particularly of infectious diseases. It is based on the hydrodynamic focusing of streams of microscopic particles (cells or microbeads) that are interrogated using laser-induced fluorescence. Flow cytometry instruments are complex, bulky and expensive, and for many years there has been extensive research into portable alternatives, primarily using microfluidics. The latter is a very appealing solution since it relies on microfabrication and, in principle, allows for the integration of the required optics and electronics into one chip. However, extending hydrodynamic focusing to microfluidic environments is not viable because: 1) It is very difficult to create a capability for three-dimensional hydrodynamic focusing in a geometry compatible with microfabrication. 2) It requires a large amount of sheath liquid, thus limiting the portability and potentially generating an equivalent volume of hazardous waste. 3) This effect works only at high flow speeds which in turn increases the cost and complexity of the optics and electronics.

An alternative to hydrodynamic focusing pioneered by Los Alamos National Laboratory and others is to use acoustic wave forces on the flowing particles (or cells) and confine them to a single flow line. An ultrasound standing wave field will move suspended particles toward either the pressure nodes or the pressure antinodes depending on the density and compressibility of the particles and medium (Fig. 1). The coupling of the acoustic force to the entire microfluidic platform also allows it to span hundreds of micron-sized fluidic channels simultaneously. Moreover, the forces can be spatially decoupled to strengthen primary radiation forces in one dimension and reduce those in other directions.

As shown schematically (cross-section) in Figure 1, Sandia researchers have recently demonstrated acoustic focusing of flowing

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particles in a silicon microfluidic chip with performance sufficient to satisfy most flow cytometry applications. A piezoelectric transducer (PZT) is integrated with a silicon microchannel of square cross section and low roughness. The microfluidic channel and corresponding through-wafer ports were fabricated using a two-step deep reactive ion etching process. The channel dimensions (~210 µm width and height) were chosen such that they set up acoustic standing waves of one-half wavelength both laterally and vertically within the cavity when actuated at 3.5 MHz.

A key aspect of this accomplishment was the development of a 2-D finite element model to predict both the location and strength of the acoustic nodes in the microchannel. The model is a dramatic improvement over prior work in that an accurate prediction of the focusing behavior is now possible. Unlike previous analytic models that are extensions of one-dimensional models, this approach captures the acoustic coupling in both the lateral and vertical directions to reveal the nodal behavior as a function of the model parameters such as input frequency. This model has been used to aid in analysis and improvement of device performance. Typical performance of such devices is shown in Fig. 2 where acoustic focusing occurs both laterally and vertically.

The reduced cost and simplification of operation of a miniature flow cytometer will enable the system to be fielded in clinical settings around the world, especially in remote locations and combat environments where trained technicians are unavailable. This would greatly increase the potential for early detection and diagnostics of pathogens, both endemic to a population and those deriving from bioterrorism.

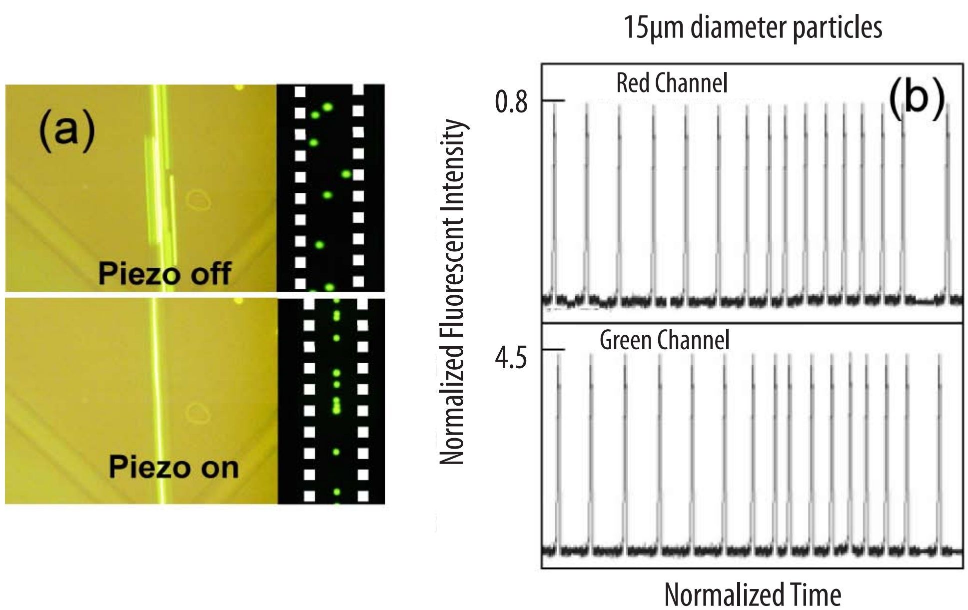

Figure 2: (a) A micrograph showing fluorescent beads when the acoustic transducer is turned on and off; (b) Uniform fluorescence intensity of two-color fluorescent beads flowing under acoustic focusing. Each spike corresponds to one bead passing through the laser beam.

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National Nuclear Security Administration

02/2009

Microelectronics and Microsystems
Optical Military Systems

Adaptive Optical Systems

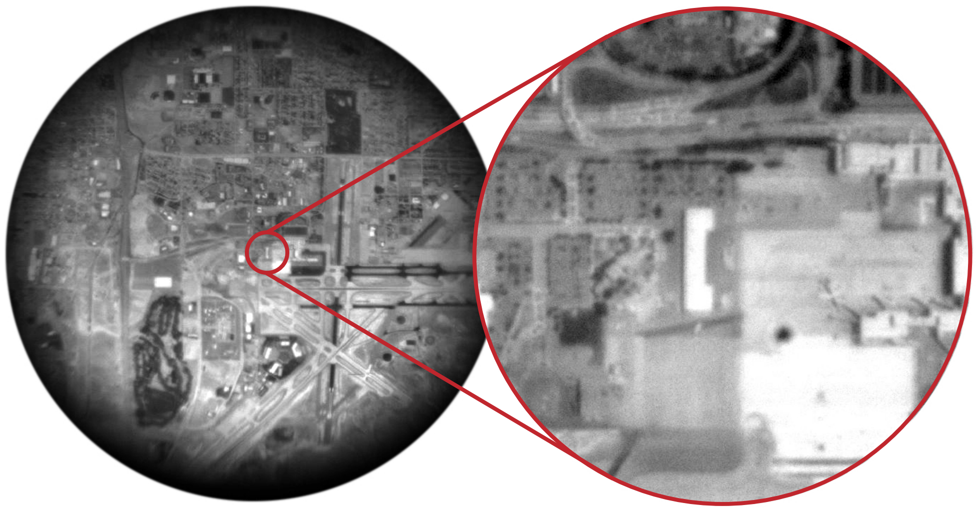

Figure 1: 8X zoom images using adaptive polymer lens rifle scope developed jointly with Holochip, Inc., for the Army's Armament Research Development and Engineering Center. There is no longitudinal motion or additional optics flipped into the optical train, as is currently done in conventional zoom systems.

Sandia technologies provide innovative imaging capabilities for situational awareness in the field

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Adaptive optical systems have been in use for over 30 years, mainly to correct atmospheric turbulence in ground-based telescopes or to improve the spatial mode and power of lasers. More recently, Sandia has led the innovation of using adaptive elements, such as deformable mirrors and spatial light modulators, to increase the resolution, magnification, field-of-view, or spectral bandwidth of imaging systems. Integration of electronically-controllable elements into a conventional lens or telescope system can increase performance or add flexibility while reducing size, weight, and power requirements. Sandia's work has supported the Defense Advanced Research Projects Agency (DARPA), the Air Force Research Laboratory (AFRL), the Office of Naval Research (ONR), and the Missile Defense Agency, and has been referenced in the development of commercially available adaptive microscopes and transmissive spatial light modulators.

An example of adaptive optical technology is shown in Figure 1, where an 8X change in magnification in a rifle scope is performed without the need for longitudinal mechanical motion, as is done in a conventional zoom lens. Instead of moving lenses, the adaptive optical zoom uses micro-opto-electro-mechanical systems, such as adaptive polymer lenses or segmented micro-electro-mechanical mirrors, to change the magnification. This concept can also be used with Sandia-developed ultralight thin-film mirrors or carbon fiber reinforced polymer mirrors for ground and space applications that require larger apertures. A telescope is now being developed that uses these variable radius mirrors to increase situational awareness while maintaining ultra-high resolution, or to improve rendezvous and docking capability. Adaptive optical zoom is ideal for applications which require both a wide field-of-view and the ability to quickly transition to high resolution for identification.

Working closely with AFRL and the Naval Research Laboratory, Sandia has also developed foveated imaging, where bulky fisheye lenses are replaced with compact, lightweight, wide field-of-view optical systems. Foveated imaging provides a

Sandia National Laboratories

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wide field-of-view (120º or more) from an extremely compact system. Rather than adding glass lenses to increase the field-of-view, as is normally done in wide-field lenses, a 1280x1024 liquid crystal spatial light modulator (SLM) is used to correct aberrations over a small area within the wider field-of-view (Figure 2). Thus, the system maintains diffraction-limited performance over a selected area of interest, with lower resolution in the perifery, similar to the human fovea.

Foveated systems are currently being developed for small unmanned aerial vehicles, where the size and weight of conventional "fish-eye" lenses are too great. DARPA based their Bio-Optic Synthetic Systems (BOSS) program, in part, on Sandia's technology. In the fielded system shown in Figure 2, the length of the lens was reduced from 19 cm to 7 cm and the volume of glass in the lens was reduced by a factor of ten. This system maintained high imaging quality out to 120 º. Foveated zoom systems utilizing MEMS mirrors are also being developed jointly with Lockheed Martin for acquisition, discrimination, and tracking. These reflective systems can quickly toggle between wide and narrow fields-of-view, magnifying any area of interest within the wider field. When zoomed-in, they can optically track a target without slewing the entire system. Thus, a foveated zoom system can survey a wide area, zoom-in quickly on multiple potential threats for discrimination, and track a target in near real-time.

In summary, adaptive optics has allowed Sandia researchers to transcend conventional glass optical systems and improve capability in many applications of interest to the military. In the case of optical zoom, these technologies allow a user to increase the resolution over an area-of-interest in near real-time and may eventually eliminate the need for gimbaled or multiple camera systems commonly used for acquisition and tracking.

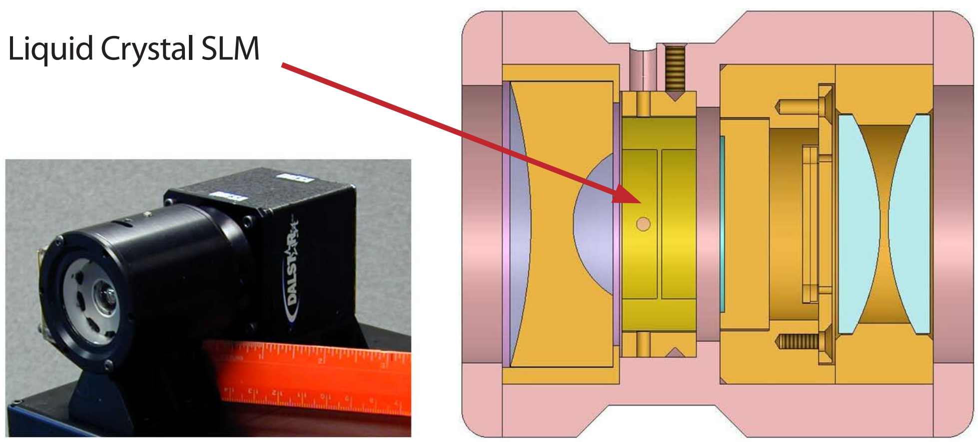

Figure 2: Foveated imaging lens developed under DARPA BOSS. The lens houses a liquid crystal spatial light modulator (developed for Sandia by Boulder Nonlinear Systems and the University of Central Florida) to dynamically correct aberrations at any point.

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National Nuclear Security Administration

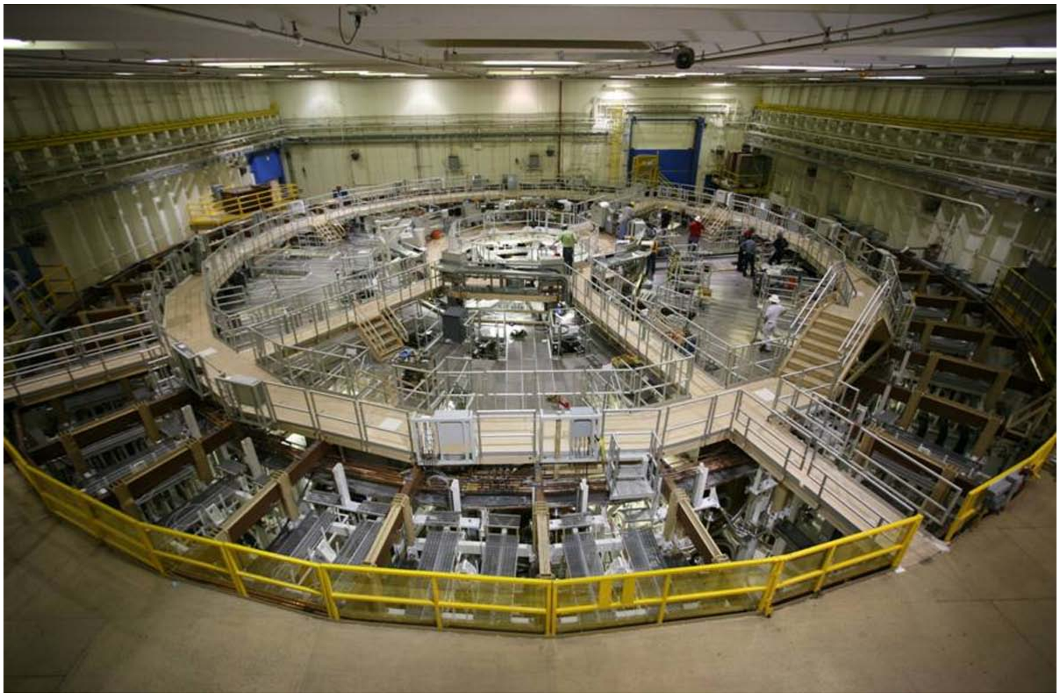
02/2009

Innovation at the Interface of Science and Engineering: The Capability Advantage

SANDIA NATIONAL LABORATORIES

Pulsed Power and *Z* Facility

The long-range goal of Sandia's pulsed power program is to provide a high-yield fusion capability for stockpile stewardship and energy applications.



Overhead view of the gymnasium-sized refurbished *Z* facility.

A technician builds an array of tungsten wires for a *Z* experiment that produces x-rays from a z-pinch implosion. Each wire is 1/10 the thickness of a human hair.

Z: The World's Largest Pulsed Power Driver

Sandia National Laboratories is the world leader in using pulsed power drivers for achieving high energy density plasmas in the laboratory. Pulsed power offers an efficient, inexpensive, and unique approach to achieving high-energy-density conditions. As the world's largest pulsed power driver, ***Z*** enables scientists to routinely perform and diagnose experiments designed to address nuclear weapon issues in the areas of dynamic material properties, secondary assessment, and nuclear survivability. The ***Z*** facility also enables scientists to access experimental conditions of interest for fundamental science in areas such as planetary physics, material properties, and laboratory astrophysics. Notably, pulsed power drivers also offer promise for achieving thermonuclear fusion ignition and high yield, which could provide a clean and abundant long-term energy source for the nation and the world.

Impressive Contributions to Stockpile Stewardship

Sandia's flagship pulsed power accelerator, ***Z***, creates extreme states of matter at pressures equivalent to that at the center of planets and at temperatures hotter than the center of the sun to evaluate weapon science phenomena. ***Z***'s unique strength is its ability to produce numerous x-rays, large plasma environments, and controlled high pressures. The ***Z*** Facility supports the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program (SSP) by providing data to

- validate simulation codes and models for material properties, radiation transport, and complex hydrodynamics
- assess target design for high-yield advanced concepts with pulsed power and fusion ignition on the National Ignition Facility
- evaluate the performance of weapon components subjected to intense x-ray environments.

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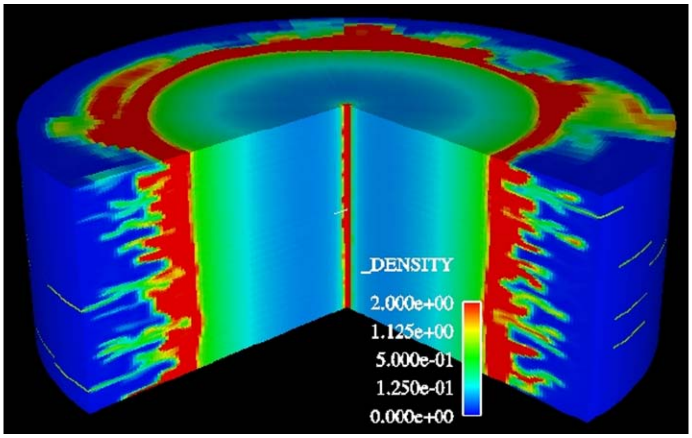


An example simulation of a Z-pinch implosion using the mass inflow model, illustrating the highly 3D nature of the pinch. (Sandia National Laboratories)

Z's Versatile Research Capabilities

Z data on the effect of electromagnetic pulse signals on test objects for Sandia's radiation effects mission have provided new insight for code models. A record neutron yield was obtained in an ignition-scale capsule with a beryllium shell. ***Z*** 's unique material property capability, developed in 1998, routinely achieves accuracies of a few percent and has been used to obtain data for deuterium, for plutonium to address pit aging, and for beryllium and high-density carbon to constrain the acceptable target design space for ignition. Exceptionally high-quality radiographic images of a wire array implosion, the imploded core of a fusion capsule, and features in a weapon secondary have been obtained.

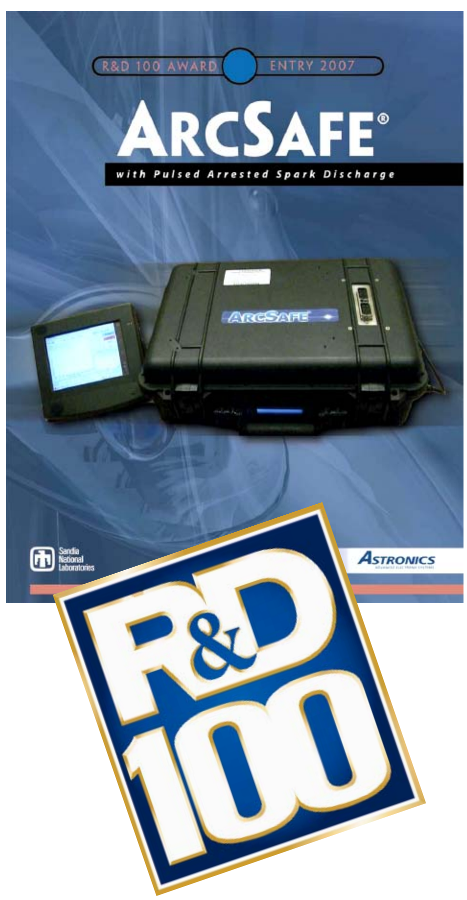
Enhancing Public Safety

Sandia's long-term expertise in pulsed power has been applied to public safety concerns. Pulsed Arrested Spark Discharge (PASD), a patented electrical wiring diagnostic developed for the Federal Aviation Administration, locates wiring insulation defects in commercial aircraft. Sandia's research in lightning and electrostatic discharge safety for stockpile facilities led to the assessment that indirect lightning was the probable cause of the Sago mine explosion near Buchhannon, W. VA. Pulsed power has provided for irradiation of the U.S. mail in response to bio-terrorism attacks.

Recognition for Innovative Work

Sandia's efforts in pulsed power technology and the ***Z*** Facility have earned numerous honors.

- Pulsed power technology received R&D100 awards for PBFA II (***Z*** 's predecessor), a photonic high-speed data recorder, and an aircraft wiring diagnostic.
- ARCSAFE® with PASD received a 2007 R&D 100 award and the 2007 Federal Laboratory Consortium Interagency Partnership Award for Excellence.



- *Industry Week* declared ***Z*** one of the top 25 technologies of 1997.
- *Discovery* magazine listed neutrons on ***Z*** as one of the top 100 Science Stories of 2003.
- NNSA Weapons Program Awards of Excellence have been received for ***Z*** refurbishment project management, implementation methods to measure material properties accurately, advanced downhole radiography, z-pinch physics x-ray sources, and the plutonium experiments.

Sandia researchers, several who are professional society fellows, have also earned many honors such as IEEE Erwin Marx and Peter Haas Awards, the E.O. Lawrence Award from DOE, the Hannes Alfven Award from the European Physical Society, the American Physical Society Shock Compression Award, and fellowship in the National Academy of Engineering.

A Promising Future

In September 2007, ***Z*** shook the ground for the first time since 2006 when the facility was taken off line for a complete upgrade. The year-long ***Z*** Refurbishment (***ZR***) was completed in 2007 to extend its life by replacing outdated components to enhance reliability and precision, allow pulse-shape flexibility, increase diagnostic access, and improve high-energy performance.

Now capable of storing twice the energy as the previous architecture, the ***ZR*** project goals were to increase facility utilization via the capacity to perform more shots, improve overall precision and pulse shape variability for better reproducibility and data quality, and increase delivered current allowing for additional performance. The improvements will enhance Sandia's pulsed power capabilities well into the next decade.

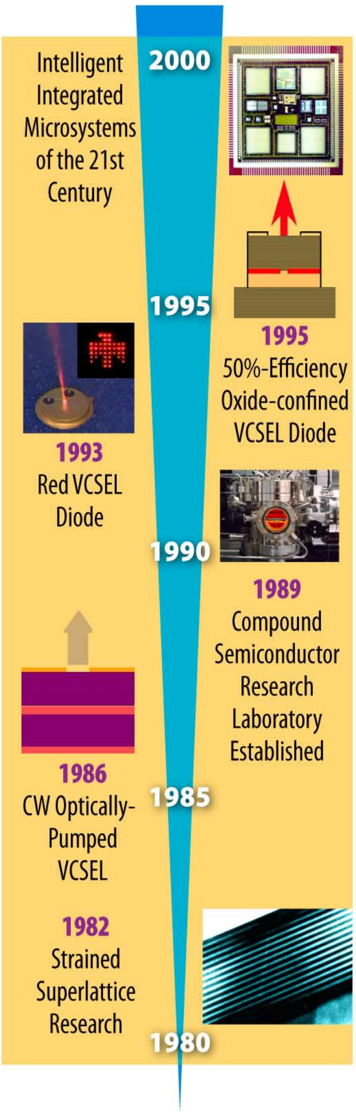
Innovation at the Interface of Science and Engineering: The Capability Advantage

SANDIA NATIONAL LABORATORIES

Nanoscience and Nanotechnology

Integration is the key to unlocking the promise of nanotechnology

Sustained Investment



Sandia's prowess in microsystems and microelectronics builds on sustained investment over several decades. The Discovery Platforms™ described here are some of the fruit of that investment. Realizing the promise of nanotechnology will require similar long-term commitment.

http://cint.lanl.gov/

Center for Integrated Nanotechnologies (CINT)

CINT, a partnership between Los Alamos and Sandia National Laboratories, is a focal point for Sandia's current research in nanoscience and nanotechnology. CINT is a Department of Energy/Office of Science Nanoscale Science Research Center operating as a national user facility devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials.

The distinguishing characteristic of CINT is its emphasis on exploring the path from scientific discovery to the integration of nanostructures into the micro and macro worlds. Integration itself is key to the exploitation of nanomaterials, and the scientific challenges that it poses are at the heart of CINT's mission.

Sandia has Performed Nanoscience Research Longer Than the Word "Nanotechnology" has Been Around

Nanotechnology refers to the manipulation or assembly of individual atoms, molecules, or molecular clusters into structures with dimensions in the 1-to 100-nanometer range to create materials and devices with new. For comparison, a human hair is about 10,000 nanometers thick.

Sandia's work in nanoscience and nanotechnology dates back more than 20 years, as evidenced by our leadership in nanoscience and nanotechnology of compound semiconductors involving nanowires and quantum dots, nanoscale structures for optimizing light extraction from semiconductor-based devices, and nanoscale control of materials for quantum computing and fundamental studies of highly correlated electron systems.

Sandia National Laboratories

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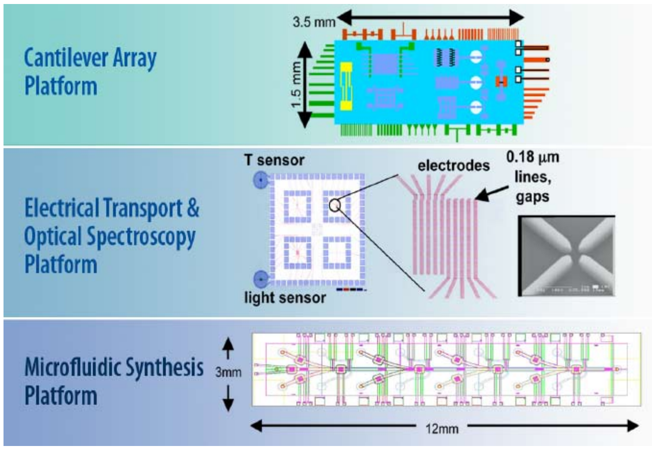
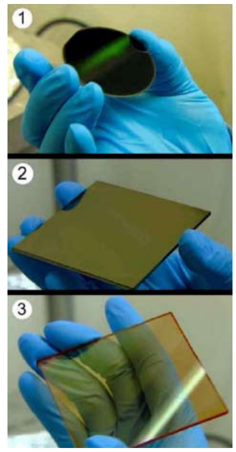


CINT's Discovery Platforms™



Examples of various nanoparticle thin films.
(1) A gold nanoparticle film on 2×2″ silicon wafer.
(2) A magnetic nanoparticle film on acrylic plate.
(3) A semiconductor nanoparticle film on acrylic plate.

Impacts on the Nanoscale

Discovery Platforms

CINT's Discovery Platforms™ are micro-labs for nanoscience exploration, and they provide platforms for user-inspired problems in areas such as mechanics, optics, electronics, and fluidics. They stimulate, interrogate, and exploit nanoscale materials in a microsystem environment. The Discovery Platforms™ (shown in the figure above) have been fabricated and are undergoing in-house testing, characterization, and integration.

Nanotechology Simulations

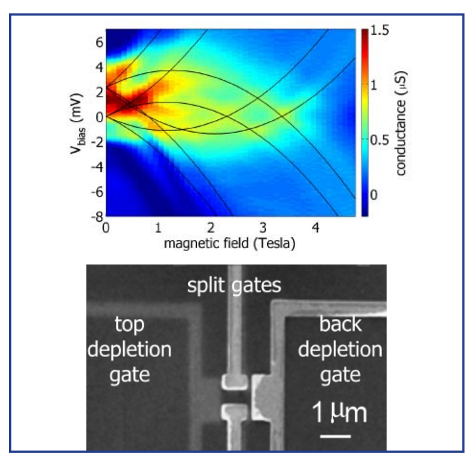
Researchers at Sandia have discovered that nanotechnology simulations provide researchers with more detailed results than experiments used alone. For example, one simulation demonstrated that a tiny but significant amount of material had transferred onto the tip of an atomic force microscope as it probed the self-assembled monolayer coating on a microsystem. Researchers discovered that the probe tip changed something infinitesimally small on the surface of the material, and it was almost not noticeable. But the property of the coating became very different. Laboratory observation could not identify the cause of the property change, but computer simulations explained the results.

Self-Assemby Process Fabricating Tailored Thin Films

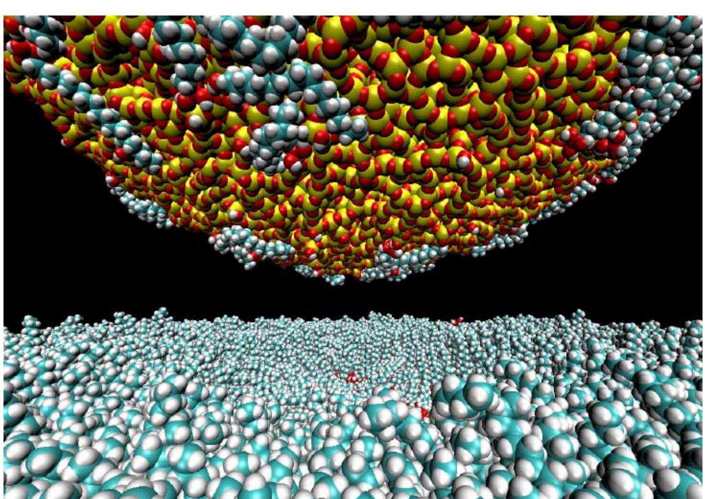
Many of today's technologies and products, including semiconductor devices, consumer electronics, and high-performance optical coatings, depend on the ability to produce high-quality thin films. Researchers at Sandia developed a wet-solution-based process employing self-assembly as a new method to produce optical and electrical thin films. This simple, economical nanotechnology driven coating process enables the development of thin films with nanoscale architectures and unique properties unattainable by any other processing method. Elegant, simple, and with more options for development and manufacturing than conventional coating processes such as chemical vapor deposition or sputtering, Sandia's technology involves chemical synthesis of mono-disperse nanoparticles with controlled chemical composition, particle size, shape, and their further assembly into engineered nanoparticle composite films.

Quantum Electron Transport

Quantum mechanical phenomena become observable only at the nanoscale but are of significant interest in the pursuit of quantum computing. Sandia scientists have combined the growth of GaAs/AlGaAs heterostructures of world-class structural and compositional purity with nanoscale fabrication techniques to fabricate two quantum wires separated by a mere 7.5 nm. Measurements on these wires reveal details about how electrons tunnel from one wire to the other and provide a significant test of theories of such systems.



Tunneling between independently contacted quantum wires provides information about energy and momentum of electrons traveling through one-dimensional systems.



"People view modeling and simulation as a critical component of nanoscience."
Eliot Fang

Left: Rendering of Sandia simulations by Michael Chandross demonstrates significant transfer of material to the probe tip of an atomic force microscope.

SANDIA NATIONAL LABORATORIES

Microsystems Engineering for Strategic Applications (MESA)

MESA Represents Sandia's Vision for the Future of Engineering

"As the last century ended, this Laboratory chose a path to a greater future. We chose to establish a unique, world-class facility that would enable the nation's security to have an anchor in unquestioned technological leadership—leadership in the synthesis of the unlimited potential of integrated microsystems, the awesome power of modeling and simulation through advanced supercomputing, and an engineering design environment where the nation's finest will be empowered and challenged and the best solutions for national security will be developed and realized." - *Thomas O. Hunter, Sandia President and Laboratories Director*

MESA is the only facility in the world that combines silicon processing with fabrication of compound-semiconductor devices under one roof.

MESA Makes It Real

The Microsystems Engineering for Strategic Applications (MESA) Complex represents the essential facilities and equipment to design, develop, manufacture, integrate, and qualify microsystems for the nation's national security needs that cannot or should not be made in industry—either because the low volumes required for these applications are not profitable for the private sector or because of stringent security requirements for such high-consequence systems as nuclear warheads.

Microsystems extend the information processing of silicon integrated circuits to add functions such as sensing, actuation, and communication—all integrated within a single package. The MESA Complex integrates the numerous scientific, engineering, and computational disciplines necessary to produce functional, robust, integrated microsystems at the center of Sandia's investment in microsystems research, development, and prototyping activities. This suite of facilities encompasses approximately 400,000 square feet and includes cleanroom facilities, laboratories, and offices.

MESA Continues Sandia's Long Tradition of Delivering Custom National Security Hardware

Sandia Invention Enables Modern Microelectronics

Willis Whitfield

The Laminar Flow Clean Room was invented by Sandia's Willis Whitfield in 1962 for the assembly of precision mechanical components. It was then applied to the pharmaceutical industry to manufacture safer drugs and to medical industry to significantly lower infection rates in hospitals. The clean room was next adopted by the semiconductor industry to enable the highly complex chips that power our modern information society.

Sandia National Laboratories

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The Sole Supplier

Sandia has developed and delivered custom, radiation-hardened microelectronics to the nuclear stockpile and other national-security customers since 1975. Sandia-built integrated circuits have assured that our nuclear deterrence could not be defeated by hostile nuclear environments from potential adversaries while maintaining the safety, security, and use control of our nuclear stockpile.

Most recently, MESA is providing all the custom integrated circuits for the W76-1 stockpile life extension, including the Permafrost digital controller that forms the brains of the nuclear warhead. The U.S. Navy found that Sandia's MESA facility was the only possible supplier that could meet the demanding mission requirements for this strategic nuclear warhead.

Beyond its support for the nuclear stockpile, Sandia provides microelectronics and microsystems for satellite payloads that monitor the earth for non-proliferation activities, specifically the Global Nuclear Burst Detector that flies on Global Positioning Satellites (GPS).

Beyond Microelectronics: *Integrated Microsystems*

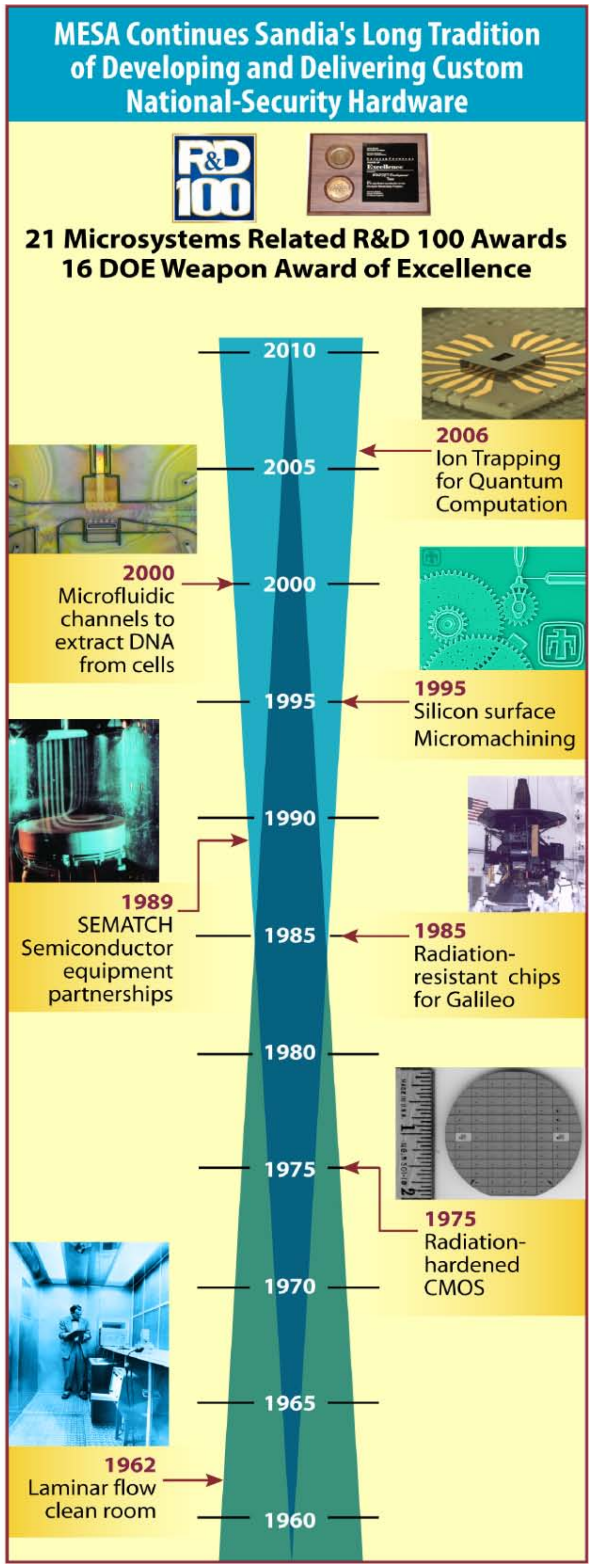
Following the events of 9-11-2001, MESA was called on to develop and deliver the key components for the PROTECT system, the nation's first permanent detection system for chemical attacks on public places such as airports and subway systems, including the San Francisco BART system and the Washington DC Metro system. Sandia's Micro-ChemLab technology continues to provides the basis for other chemical warning systems as SnifferStar, which flies on unmanned aerial vehicles. The same technology forms the basis for the MicroHound hand-held chemical detection unit for first responders and which also sniffs for drugs to support law-enforcement officials.

MESA continues to pioneer new technologies. Within the past year, MESA provided the first fully space-qualified MicroElectroMechanical Systems (MEMS) to control the temperature of nanosatellites while functioning in the radiation of space.

Sandia has developed a chip-scale atomic clock with the goal of transforming atomic clocks from laboratory rack-mounted instruments to low-power, hand-held devices that could be carried by a soldier to enable jam-proof communication and precision navigation in GPS-denied environments.

Most recently, Sandia developed the first scalable approach to quantum computation through trapped ions to one day enable massively parallel computation on a single chip rather than through rooms full of complex computer equipment.

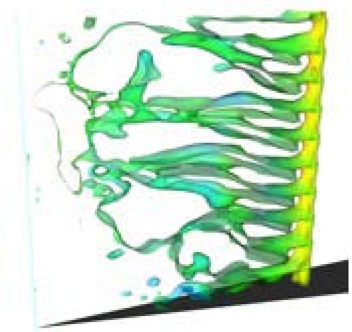
The benefits of MESA extend beyond mere hardware. As Tom Hunter's vision stated, a key aspect of MESA is to entice and invigorate some of the nation's best scientific and technical talent to apply their skills to the esoteric needs of national security. The partnership between DOE's Center for Integrated Nanotechnology (CINT) and MESA is a prototype for bringing leading-edge capabilities to the service of our nation's security.

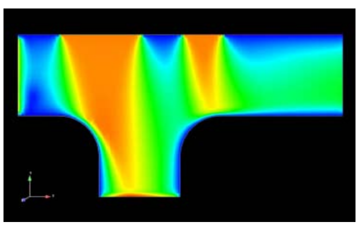


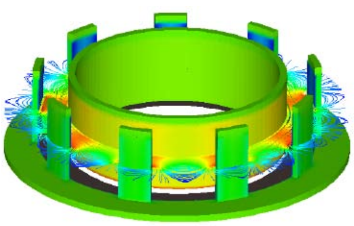
Innovation at the Interface of Science and Engineering: The Capability Advantage

SANDIA NATIONAL LABORATORIES
High-Performance Computing

Sandia has a long and distinguished history in massively parallel computing.







State-of-the-Art Computational Science Applications: (top) Understanding plasma instabilities is a critical element in achieving fusion in the laboratory. (middle) The detailed behavior of semi-conductor material when insulted with radiation is required to predict the surviv-ability of satellites and weapon systems. (bottom) Simulation is being used to optimize the magnetohydrodynamic drive of pulse power systems.

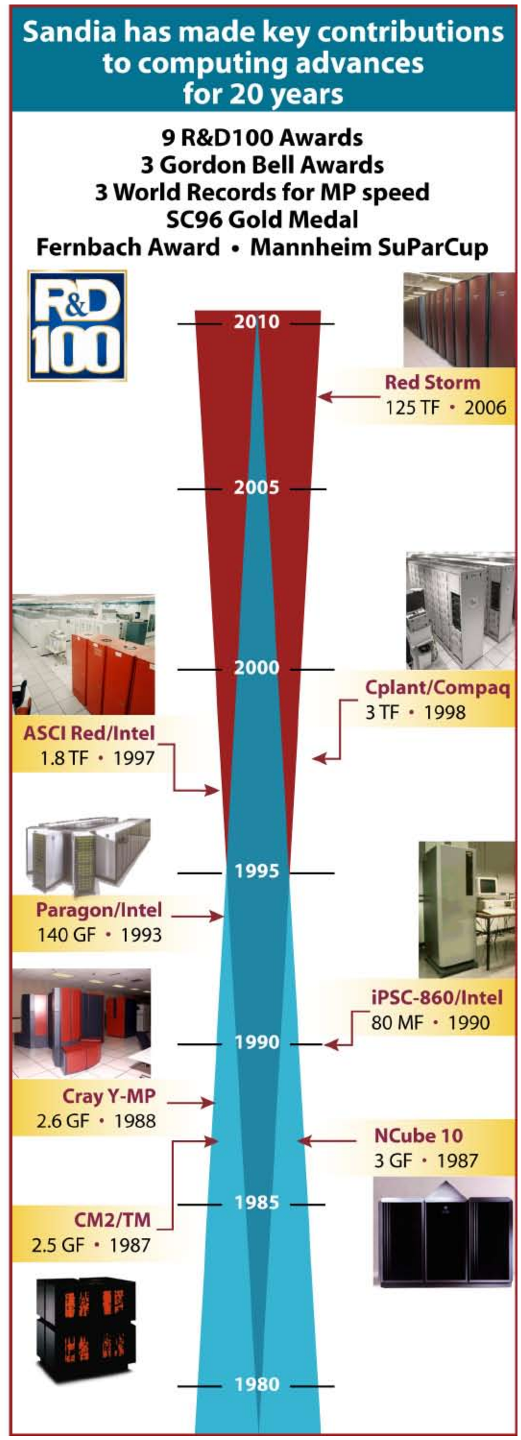
Sandia's Parallel Computing History

Sandia has a long and distinguished history in massively parallel computing. In 1987 Sandia won the inaugural Gordon Bell Prize and the Karp Challenge for showing that scientific applications could achieve thousand-fold speedups on Massively Parallel Processors (MPPs). In the late 1980s Sandia was the first national laboratory to transition all of its computing from vector supercomputers to MPPs. Since then Sandia computational scientists have won two more Gordon Bell Prizes, numerous R&D100 awards, and the Mannheim SuperCup. A Sandia partnership with Intel resulted in several world records for computational speed and the development of the world's first Teraflops supercomputer in 1997 (ASCI Red).

Sandia's work in high-performance computing (HPC) has been para-mount to the success of Advanced Simulation & Computing (ASC) at all three NNSA laboratories.

Distinguishing impacts include:

- Extremely broad set of applications ranging from materials science to mechanical response and high-energy density physics to electrical system response
- Lightweight kernel technology that formed the basis for the operating systems on the Intel Paragon, the Intel Teraflops supercomputer (ASCI Red), and Cray's XT3
- Key mathematical libraries that are used by the tri-lab HPC community (Trilinos for solving systems of equa-tions; Zoltan for load balancing; and Dakota for optimization)



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Sandia's Red Storm: The design of Red Storm facilitates cost-effective upgrades to more than 30 times beyond the serial #1 platform and has provided the foundation for the DOE Office of Science Leadership Class Petaflop computer at Oak Ridge National Laboratory. Presently, there are 36 Red Storm installations at 20 sites.

Red Storm : Balanced Performance + Time Critical Applications = Commercial Success

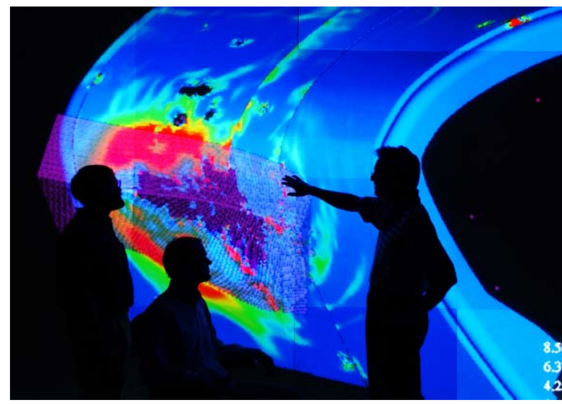
In addition, Sandia and Cray partnered with the support of the NNSA ASC program to develop Red Storm, the most successful massively parallel supercomputer to date. The goal of the design was to create a balanced supercomputer that achieves high performance on real applications. Not only did Sandia researchers play a key role in the design of Red Storm, they developed the operating system that runs the machine. The commercial version of Red Storm, XT3/4, has achieved considerable success as evidenced by its worldwide sales. Cray XT3/4 sites include the Swiss National Computing Center, DoD's Stennis Computing Center, DOE's Oak Ridge National Laboratory, National Science Foundation's Pittsburgh Supercomputing Center, DOE's National Energy Research Scientific Computing Center, and UK's Atomic Weapons Establishment.

As initially configured, Red Storm provides over 10,000 compute nodes for massively parallel computations. Application teams from the three defense laboratories are successfully using Red Storm to provide computational results in support of the NNSA Stockpile Stewardship Program.

CSRI: A Model for U.S. Competitiveness in HPC

Sandia recently opened the Computer Science Research Institute (CSRI) which brings together researchers from universities and the national laboratories in an exciting and dynamic environment to address research problems in parallel computing, computer science, computational science, and mathematics to develop new capabilities in modeling and simulation.

CSRI has become a model for government, industry, and university collaboration. HPC results from Sandia, for example, played an integral role in helping NASA understand the underlying cause of the shuttle *Columbia* accident.



Researchers at Sandia's Visualization Laboratory discuss a computer simulation and analysis showing the impact of a foam piece along the leading edge of the space shuttle *Columbia's* wing.

Sandia's Computer Science Research Institute is a focal point for collaborations. The CSRI hosts over 200 visitors per year, including over 40 summer students and faculty. Other collaborations include research projects, post-docs, sabbaticals and four to six workshops per year. See http://www.cs.sandia.gov/CSRI for more information.